Supporting information

SWISS-MODEL is an automated structure-homology modeling server that is available through the ExPASy web server. [84] The sequence for each bacteriocin was uploaded to the server followed by an automated search through the Research Collaboratory Structural Bioinformatics' (RCSB) Protein Data Bank (PDB) for a homologous peptide with an experimentally determined structure.[85] PDB coordinates of the peptide with the highest sequence-homology were used to create a structural model of each bacteriocin of interest.

1. Pneumocyclicin

A) PDB file for model of pneumocyclicin. Structure modeled after NKR-5-3B using SWISS-MODEL[84]

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TITLE     SWISS-MODEL SERVER (https://swissmodel.expasy.org)
TITLE    2 Untitled Project
EXPDTA    THEORETICAL MODEL (SWISS-MODEL SERVER)
AUTHOR    SWISS-MODEL SERVER (SEE REFERENCE IN JRNL
Records)
REVDAT   1   31-OCT-16 1MOD    1       15:24
JRNL       AUTH
M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL       AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO
CASSARINO,M.BERTONI,L.BORDOLI,
JRNL       AUTH 3 T.SCHWEDE
JRNL       TITL   SWISS-MODEL: MODELLING PROTEIN TERTIARY
AND QUATERNARY
JRNL       TITL 2 STRUCTURE USING EVOLUTIONARY
INFORMATION
JRNL       REF    NUCLEIC.ACIDS.RES                2014
JRNL       REFN                ISSN 0305-1048
JRNL       PMID   24782522
JRNL       DOI    10.1093/nar/gku340
REMARK   3 MODEL INFORMATION
REMARK   3  ENGIN   PROMOD3
REMARK   3  VERSN   1.0.1
REMARK   3  OSTAT   MONOMER
REMARK   3  OSRSN   USER
REMARK   3  GMQE    0.79
REMARK   3  QMN4    -1.18
REMARK   3  MODT    FALSE
REMARK   3
REMARK   3 TEMPLATE 1
REMARK   3  PDBID   2mp8
REMARK   3  CHAIN   A
REMARK   3  MMCIF   A
REMARK   3  PDBV    2016-10-14
REMARK   3  SMTLE   2mp8.1.A
REMARK   3  SMTLV   2016-10-19
REMARK   3  MTHD    SOLUTION NMR 0.00 A
REMARK   3  FOUND   HHblits
REMARK   3  GMQE    0.79
REMARK   3  SIM     0.40
REMARK   3  SID     43.75
REMARK   3  OSTAT   monomer
ATOM      1  N   LEU A   1       5.377  -3.179   1.001  1.00  0.75           N
ATOM      2  CA  LEU A   1       4.201  -4.013   0.852  1.00  0.75           C
ATOM      3  C   LEU A   1       4.594  -5.415   0.498  1.00  0.75           C
ATOM      4  O   LEU A   1       4.214  -6.343   1.171  1.00  0.75           O
ATOM      5  CB  LEU A   1       3.366  -3.247  -0.183  1.00  0.75           C
ATOM      6  CG  LEU A   1       2.923  -1.834   0.250  1.00  0.75           C
ATOM      7  CD1 LEU A   1       2.299  -1.181  -0.987  1.00  0.75           C
ATOM      8  CD2 LEU A   1       1.992  -1.884   1.476  1.00  0.75           C
ATOM      9  N   ALA A   2       5.395  -5.633  -0.563  1.00  0.74           N
ATOM     10  CA  ALA A   2       5.744  -6.972  -0.972  1.00  0.74           C
ATOM     11  C   ALA A   2       6.430  -7.903   0.044  1.00  0.74           C
ATOM     12  O   ALA A   2       6.047  -9.051   0.194  1.00  0.74           O
ATOM     13  CB  ALA A   2       6.627  -6.844  -2.216  1.00  0.74           C
ATOM     14  N   GLY A   3       7.421  -7.382   0.793  1.00  0.70           N
ATOM     15  CA  GLY A   3       8.158  -8.029   1.864  1.00  0.70           C
ATOM     16  C   GLY A   3       7.369  -8.184   3.141  1.00  0.70           C
ATOM     17  O   GLY A   3       7.422  -9.245   3.754  1.00  0.70           O
ATOM     18  N   THR A   4       6.617  -7.154   3.605  1.00  0.68           N
ATOM     19  CA  THR A   4       5.835  -7.268   4.852  1.00  0.68           C
ATOM     20  C   THR A   4       4.537  -8.022   4.715  1.00  0.68           C
ATOM     21  O   THR A   4       4.109  -8.717   5.636  1.00  0.68           O
ATOM     22  CB  THR A   4       5.498  -5.972   5.580  1.00  0.68           C
ATOM     23  OG1 THR A   4       4.723  -5.061   4.795  1.00  0.68           O
ATOM     24  CG2 THR A   4       6.810  -5.286   5.969  1.00  0.68           C
ATOM     25  N   LEU A   5       3.857  -7.886   3.565  1.00  0.69           N
ATOM     26  CA  LEU A   5       2.564  -8.491   3.335  1.00  0.69           C
ATOM     27  C   LEU A   5       2.699  -9.831   2.644  1.00  0.69           C
ATOM     28  O   LEU A   5       1.785 -10.649   2.684  1.00  0.69           O
ATOM     29  CB  LEU A   5       1.717  -7.595   2.398  1.00  0.69           C
ATOM     30  CG  LEU A   5       1.561  -6.136   2.860  1.00  0.69           C
ATOM     31  CD1 LEU A   5       0.936  -5.323   1.725  1.00  0.69           C
ATOM     32  CD2 LEU A   5       0.732  -5.999   4.137  1.00  0.69           C
ATOM     33  N   GLY A   6       3.851 -10.082   1.982  1.00  0.76           N
ATOM     34  CA  GLY A   6       4.101 -11.315   1.245  1.00  0.76           C
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ATOM     36  O   GLY A   6       2.784 -12.419  -0.417  1.00  0.76           O
ATOM     37  N   ILE A   7       3.238 -10.241  -0.743  1.00  0.72           N
ATOM     38  CA  ILE A   7       2.450 -10.082  -1.948  1.00  0.72           C
ATOM     39  C   ILE A   7       3.369  -9.882  -3.126  1.00  0.72           C
ATOM     40  O   ILE A   7       4.571  -9.657  -3.002  1.00  0.72           O
ATOM     41  CB  ILE A   7       1.434  -8.933  -1.898  1.00  0.72           C
ATOM     42  CG1 ILE A   7       2.105  -7.556  -1.667  1.00  0.72           C
ATOM     43  CG2 ILE A   7       0.377  -9.288  -0.829  1.00  0.72           C
ATOM     44  CD1 ILE A   7       1.134  -6.374  -1.743  1.00  0.72           C
ATOM     45  N   SER A   8       2.811  -9.971  -4.343  1.00  0.81           N
ATOM     46  CA  SER A   8       3.535  -9.703  -5.569  1.00  0.81           C
ATOM     47  C   SER A   8       3.850  -8.230  -5.753  1.00  0.81           C
ATOM     48  O   SER A   8       3.212  -7.349  -5.178  1.00  0.81           O
ATOM     49  CB  SER A   8       2.779 -10.222  -6.822  1.00  0.81           C
ATOM     50  OG  SER A   8       1.522  -9.560  -7.025  1.00  0.81           O
ATOM     51  N   THR A   9       4.847  -7.908  -6.598  1.00  0.76           N
ATOM     52  CA  THR A   9       5.165  -6.537  -6.986  1.00  0.76           C
ATOM     53  C   THR A   9       4.026  -5.881  -7.745  1.00  0.76           C
ATOM     54  O   THR A   9       3.783  -4.683  -7.608  1.00  0.76           O
ATOM     55  CB  THR A   9       6.427  -6.438  -7.829  1.00  0.76           C
ATOM     56  OG1 THR A   9       6.356  -7.284  -8.969  1.00  0.76           O
ATOM     57  CG2 THR A   9       7.624  -6.929  -7.009  1.00  0.76           C
ATOM     58  N   LYS A  10       3.278  -6.679  -8.541  1.00  0.75           N
ATOM     59  CA  LYS A  10       2.065  -6.280  -9.231  1.00  0.75           C
ATOM     60  C   LYS A  10       0.979  -5.816  -8.284  1.00  0.75           C
ATOM     61  O   LYS A  10       0.424  -4.733  -8.437  1.00  0.75           O
ATOM     62  CB  LYS A  10       1.475  -7.489 -10.008  1.00  0.75           C
ATOM     63  CG  LYS A  10       0.201  -7.170 -10.816  1.00  0.75           C
ATOM     64  CD  LYS A  10      -0.345  -8.403 -11.560  1.00  0.75           C
ATOM     65  CE  LYS A  10      -1.617  -8.103 -12.365  1.00  0.75           C
ATOM     66  NZ  LYS A  10      -2.091  -9.315 -13.077  1.00  0.75           N
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ATOM     67  N   ALA A  11       0.683  -6.620  -7.239  1.00  0.83           N
ATOM     68  CA  ALA A  11      -0.249  -6.250  -6.206  1.00  0.83           C
ATOM     69  C   ALA A  11       0.267  -5.066  -5.418  1.00  0.83           C
ATOM     70  O   ALA A  11      -0.469  -4.118  -5.190  1.00  0.83           O
ATOM     71  CB  ALA A  11      -0.520  -7.441  -5.268  1.00  0.83           C
ATOM     72  N   ALA A  12       1.563  -5.045  -5.042  1.00  0.82           N
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ATOM     76  CB  ALA A  12       3.640  -4.241  -4.032  1.00  0.82           C
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ATOM     78  CA  ALA A  13       2.195  -1.357  -7.194  1.00  0.83           C
ATOM     79  C   ALA A  13       0.747  -0.912  -7.314  1.00  0.83           C
ATOM     80  O   ALA A  13       0.409   0.278  -7.328  1.00  0.83           O
ATOM     81  CB  ALA A  13       2.736  -1.660  -8.603  1.00  0.83           C
ATOM     82  N   THR A  14      -0.174  -1.871  -7.377  1.00  0.82           N
ATOM     83  CA  THR A  14      -1.591  -1.613  -7.284  1.00  0.82           C
ATOM     84  C   THR A  14      -2.015  -1.032  -5.938  1.00  0.82           C
ATOM     85  O   THR A  14      -2.759  -0.056  -5.895  1.00  0.82           O
ATOM     86  CB  THR A  14      -2.375  -2.856  -7.592  1.00  0.82           C
ATOM     87  OG1 THR A  14      -2.158  -3.285  -8.924  1.00  0.82           O
ATOM     88  CG2 THR A  14      -3.849  -2.546  -7.539  1.00  0.82           C
ATOM     89  N   VAL A  15      -1.507  -1.562  -4.797  1.00  0.82           N
ATOM     90  CA  VAL A  15      -1.705  -0.996  -3.457  1.00  0.82           C
ATOM     91  C   VAL A  15      -1.162   0.421  -3.402  1.00  0.82           C
ATOM     92  O   VAL A  15      -1.830   1.312  -2.878  1.00  0.82           O
ATOM     93  CB  VAL A  15      -1.014  -1.776  -2.331  1.00  0.82           C
ATOM     94  CG1 VAL A  15      -1.220  -1.107  -0.947  1.00  0.82           C
ATOM     95  CG2 VAL A  15      -1.489  -3.234  -2.232  1.00  0.82           C
ATOM     96  N   VAL A  16       0.029   0.670  -3.998  1.00  0.81           N
ATOM     97  CA  VAL A  16       0.653   1.983  -4.145  1.00  0.81           C
ATOM     98  C   VAL A  16      -0.275   2.981  -4.808  1.00  0.81           C
ATOM     99  O   VAL A  16      -0.485   4.082  -4.301  1.00  0.81           O
ATOM    100  CB  VAL A  16       1.950   1.935  -4.953  1.00  0.81           C
ATOM    101  CG1 VAL A  16       2.437   3.331  -5.386  1.00  0.81           C
ATOM    102  CG2 VAL A  16       3.065   1.233  -4.159  1.00  0.81           C
ATOM    103  N   ASN A  17      -0.914   2.626  -5.934  1.00  0.79           N
ATOM    104  CA  ASN A  17      -1.861   3.512  -6.590  1.00  0.79           C
ATOM    105  C   ASN A  17      -3.042   3.877  -5.713  1.00  0.79           C
ATOM    106  O   ASN A  17      -3.482   5.023  -5.674  1.00  0.79           O
ATOM    107  CB  ASN A  17      -2.429   2.875  -7.872  1.00  0.79           C
ATOM    108  CG  ASN A  17      -1.359   2.837  -8.948  1.00  0.79           C
ATOM    109  OD1 ASN A  17      -0.439   3.655  -8.994  1.00  0.79
O
ATOM    110  ND2 ASN A  17      -1.511   1.884  -9.894  1.00  0.79
N
ATOM    111  N   LEU A  18      -3.578   2.899  -4.973  1.00  0.77           N
ATOM    112  CA  LEU A  18      -4.656   3.130  -4.047  1.00  0.77           C
ATOM    113  C   LEU A  18      -4.326   3.958  -2.838  1.00  0.77           C
ATOM    114  O   LEU A  18      -5.012   4.924  -2.531  1.00  0.77           O
ATOM    115  CB  LEU A  18      -5.147   1.785  -3.535  1.00  0.77           C
ATOM    116  CG  LEU A  18      -5.679   0.876  -4.631  1.00  0.77           C
ATOM    117  CD1 LEU A  18      -6.041  -0.415  -3.933  1.00  0.77           C
ATOM    118  CD2 LEU A  18      -6.911   1.495  -5.276  1.00  0.77           C
ATOM    119  N   ILE A  19      -3.238   3.681  -2.122  1.00  0.74           N
ATOM    120  CA  ILE A  19      -2.875   4.478  -0.970  1.00  0.74           C
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ATOM    124  CG1 ILE A  19      -0.507   3.763  -1.149  1.00  0.74           C
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ATOM    126  CD1 ILE A  19       0.722   3.194  -0.495  1.00  0.74           C
ATOM    127  N   SER A  20      -1.979   6.094  -2.587  1.00  0.78           N
ATOM    128  CA  SER A  20      -1.607   7.377  -3.157  1.00  0.78           C
ATOM    129  C   SER A  20      -2.798   8.206  -3.571  1.00  0.78           C
ATOM    130  O   SER A  20      -2.793   9.425  -3.421  1.00  0.78           O
ATOM    131  CB  SER A  20      -0.737   7.242  -4.434  1.00  0.78           C
ATOM    132  OG  SER A  20       0.600   6.819  -4.148  1.00  0.78           O
ATOM    133  N   ALA A  21      -3.827   7.575  -4.175  1.00  0.74           N
ATOM    134  CA  ALA A  21      -4.995   8.260  -4.692  1.00  0.74           C
ATOM    135  C   ALA A  21      -6.026   8.600  -3.641  1.00  0.74           C
ATOM    136  O   ALA A  21      -6.664   9.649  -3.666  1.00  0.74           O
ATOM    137  CB  ALA A  21      -5.690   7.370  -5.742  1.00  0.74           C
ATOM    138  N   TYR A  22      -6.242   7.664  -2.711  1.00  0.69           N
ATOM    139  CA  TYR A  22      -7.238   7.764  -1.686  1.00  0.69           C
ATOM    140  C   TYR A  22      -6.706   8.543  -0.515  1.00  0.69           C
ATOM    141  O   TYR A  22      -5.517   8.547  -0.226  1.00  0.69           O
ATOM    142  CB  TYR A  22      -7.576   6.371  -1.133  1.00  0.69           C
ATOM    143  CG  TYR A  22      -8.435   5.564  -2.034  1.00  0.69           C
ATOM    144  CD1 TYR A  22      -7.989   5.135  -3.287  1.00  0.69           C
ATOM    145  CD2 TYR A  22      -9.715   5.190  -1.619  1.00  0.69           C
ATOM    146  CE1 TYR A  22      -8.858   4.516  -4.179  1.00  0.69           C
ATOM    147  CE2 TYR A  22     -10.598   4.563  -2.507  1.00  0.69
C
ATOM    148  CZ  TYR A  22     -10.178   4.290  -3.813  1.00  0.69           C
ATOM    149  OH  TYR A  22     -11.011   3.718  -4.783  1.00  0.69
O
ATOM    150  N   SER A  23      -7.623   9.195   0.213  1.00  0.66           N
ATOM    151  CA  SER A  23      -7.266  10.130   1.263  1.00  0.66           C
ATOM    152  C   SER A  23      -7.506   9.530   2.624  1.00  0.66           C
ATOM    153  O   SER A  23      -6.588   9.223   3.388  1.00  0.66           O
ATOM    154  CB  SER A  23      -8.132  11.409   1.143  1.00  0.66           C
ATOM    155  OG  SER A  23      -7.847  12.060  -0.092  1.00  0.66           O
ATOM    156  N   THR A  24      -8.786   9.355   2.990  1.00  0.68           N
ATOM    157  CA  THR A  24      -9.224   8.781   4.253  1.00  0.68           C
ATOM    158  C   THR A  24      -8.760   7.358   4.431  1.00  0.68           C
ATOM    159  O   THR A  24      -8.978   6.525   3.558  1.00  0.68           O
ATOM    160  CB  THR A  24     -10.741   8.794   4.359  1.00  0.68           C
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O
ATOM    162  CG2 THR A  24     -11.265   8.198   5.674  1.00  0.68
C
ATOM    163  N   VAL A  25      -8.165   7.015   5.597  1.00  0.71           N
ATOM    164  CA  VAL A  25      -7.587   5.701   5.847  1.00  0.71           C
ATOM    165  C   VAL A  25      -8.601   4.582   5.658  1.00  0.71           C
ATOM    166  O   VAL A  25      -8.359   3.625   4.936  1.00  0.71           O
ATOM    167  CB  VAL A  25      -7.017   5.624   7.260  1.00  0.71           C
ATOM    168  CG1 VAL A  25      -6.364   4.249   7.516  1.00  0.71           C
ATOM    169  CG2 VAL A  25      -5.966   6.735   7.448  1.00  0.71           C
ATOM    170  N   THR A  26      -9.813   4.725   6.220  1.00  0.70           N
ATOM    171  CA  THR A  26     -10.935   3.794   6.066  1.00  0.70           C
ATOM    172  C   THR A  26     -11.333   3.558   4.630  1.00  0.70           C
ATOM    173  O   THR A  26     -11.600   2.427   4.214  1.00  0.70           O
ATOM    174  CB  THR A  26     -12.149   4.289   6.835  1.00  0.70           C
ATOM    175  OG1 THR A  26     -11.798   4.409   8.205  1.00  0.70
O
ATOM    176  CG2 THR A  26     -13.340   3.323   6.743  1.00  0.70
C
ATOM    177  N   ALA A  27     -11.342   4.621   3.808  1.00  0.74           N
ATOM    178  CA  ALA A  27     -11.603   4.546   2.389  1.00  0.74           C
ATOM    179  C   ALA A  27     -10.510   3.767   1.660  1.00  0.74           C
ATOM    180  O   ALA A  27     -10.801   2.930   0.803  1.00  0.74           O
ATOM    181  CB  ALA A  27     -11.723   5.971   1.815  1.00  0.74           C
ATOM    182  N   VAL A  28      -9.226   4.009   2.033  1.00  0.75           N
ATOM    183  CA  VAL A  28      -8.062   3.249   1.578  1.00  0.75           C
ATOM    184  C   VAL A  28      -8.154   1.784   1.906  1.00  0.75           C
ATOM    185  O   VAL A  28      -8.015   0.928   1.047  1.00  0.75           O
ATOM    186  CB  VAL A  28      -6.723   3.712   2.138  1.00  0.75           C
ATOM    187  CG1 VAL A  28      -5.575   2.947   1.470  1.00  0.75           C
ATOM    188  CG2 VAL A  28      -6.475   5.149   1.728  1.00  0.75           C
ATOM    189  N   ILE A  29      -8.454   1.421   3.154  1.00  0.70           N
ATOM    190  CA  ILE A  29      -8.473   0.026   3.559  1.00  0.70           C
ATOM    191  C   ILE A  29      -9.472  -0.801   2.767  1.00  0.70           C
ATOM    192  O   ILE A  29      -9.167  -1.893   2.276  1.00  0.70           O
ATOM    193  CB  ILE A  29      -8.832  -0.062   5.025  1.00  0.70           C
ATOM    194  CG1 ILE A  29      -7.771   0.637   5.895  1.00  0.70           C
ATOM    195  CG2 ILE A  29      -8.978  -1.536   5.461  1.00  0.70           C
ATOM    196  CD1 ILE A  29      -8.316   0.898   7.297  1.00  0.70           C
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ATOM    197  N   SER A  30     -10.686  -0.250   2.580  1.00  0.77           N
ATOM    198  CA  SER A  30      -11.761  -0.880   1.832  1.00  0.77           C
ATOM    199  C   SER A  30      -11.417  -1.109   0.391  1.00  0.77           C
ATOM    200  O   SER A  30      -11.705  -2.169  -0.170  1.00  0.77           O
ATOM    201  CB  SER A  30      -13.046  -0.030   1.849  1.00  0.77           C
ATOM    202  OG  SER A  30      -13.559   0.025   3.179  1.00  0.77           O
ATOM    203  N   ILE A  31     -10.777  -0.125  -0.263  1.00  0.73           N
ATOM    204  CA  ILE A  31      -10.334  -0.311  -1.625  1.00  0.73           C
ATOM    205  C   ILE A  31      -9.185  -1.302  -1.761  1.00  0.73           C
ATOM    206  O   ILE A  31      -9.217  -2.178  -2.621  1.00  0.73           O
ATOM    207  CB  ILE A  31      -10.034   0.994  -2.337  1.00  0.73           C
ATOM    208  CG1 ILE A  31       -9.939   0.766  -3.857  1.00  0.73           C
ATOM    209  CG2 ILE A  31       -8.790   1.691  -1.751  1.00  0.73           C
ATOM    210  CD1 ILE A  31      -11.276   0.537  -4.562  1.00  0.73           C
ATOM    211  N   VAL A  32       -8.147  -1.240  -0.893  1.00  0.78           N
ATOM    212  CA  VAL A  32       -6.986  -2.107  -1.005  1.00  0.78           C
ATOM    213  C   VAL A  32       -7.378  -3.544  -0.794  1.00  0.78           C
ATOM    214  O   VAL A  32       -6.976  -4.430  -1.554  1.00  0.78           O
ATOM    215  CB  VAL A  32       -5.833  -1.742  -0.078  1.00  0.78           C
ATOM    216  CG1 VAL A  32       -4.619  -2.582  -0.483  1.00  0.78
C
ATOM    217  CG2 VAL A  32       -5.381  -0.279  -0.231  1.00  0.78
C
ATOM    218  N   GLY A  33       -8.249  -3.792   0.197  1.00  0.76           N
ATOM    219  CA  GLY A  33       -8.784  -5.112   0.474  1.00  0.76           C
ATOM    220  C   GLY A  33       -9.632  -5.702  -0.626  1.00  0.76           C
ATOM    221  O   GLY A  33       -9.616  -6.911  -0.843  1.00  0.76           O
ATOM    222  N   ALA A  34      -10.368  -4.853  -1.374  1.00  0.76           N
ATOM    223  CA  ALA A  34      -11.126  -5.227  -2.554  1.00  0.76
C
ATOM    224  C   ALA A  34      -10.250  -5.649  -3.720  1.00  0.76           C
ATOM    225  O   ALA A  34      -10.588  -6.547  -4.488  1.00  0.76           O
ATOM    226  CB  ALA A  34      -12.033  -4.057  -2.997  1.00  0.76
C
ATOM    227  N   ILE A  35       -9.103  -4.980  -3.889  1.00  0.72           N
ATOM    228  CA  ILE A  35       -8.169  -5.275  -4.947  1.00  0.72           C
ATOM    229  C   ILE A  35       -7.242  -6.443  -4.658  1.00  0.72           C
ATOM    230  O   ILE A  35       -7.026  -7.307  -5.509  1.00  0.72           O
ATOM    231  CB  ILE A  35       -7.339  -4.047  -5.188  1.00  0.72           C
ATOM    232  CG1 ILE A  35       -8.143  -2.848  -5.753  1.00  0.72           C
ATOM    233  CG2 ILE A  35       -6.197  -4.350  -6.150  1.00  0.72           C
ATOM    234  CD1 ILE A  35       -9.004  -3.078  -7.000  1.00  0.72           C
ATOM    235  N   THR A  36       -6.631  -6.510  -3.458  1.00  0.74           N
ATOM    236  CA  THR A  36       -5.709  -7.595  -3.143  1.00  0.74           C
ATOM    237  C   THR A  36       -6.442  -8.860  -2.755  1.00  0.74           C
ATOM    238  O   THR A  36       -5.874  -9.949  -2.817  1.00  0.74           O
ATOM    239  CB  THR A  36       -4.712  -7.275  -2.032  1.00  0.74           C
ATOM    240  OG1 THR A  36       -5.359  -6.851  -0.841  1.00  0.74
O
ATOM    241  CG2 THR A  36       -3.790  -6.127  -2.459  1.00  0.74
C
ATOM    242  N   GLY A  37       -7.732  -8.748  -2.361  1.00  0.77           N
ATOM    243  CA  GLY A  37       -8.578  -9.876  -1.996  1.00  0.77           C
ATOM    244  C   GLY A  37       -8.225 -10.445  -0.650  1.00  0.77           C
ATOM    245  O   GLY A  37       -8.328 -11.640  -0.409  1.00  0.77           O
ATOM    246  N   VAL A  38       -7.764  -9.577   0.267  1.00  0.66           N
ATOM    247  CA  VAL A  38       -7.295  -9.989   1.572  1.00  0.66           C
ATOM    248  C   VAL A  38       -7.358  -8.784   2.498  1.00  0.66           C
ATOM    249  O   VAL A  38       -7.213  -7.641   2.077  1.00  0.66           O
ATOM    250  CB  VAL A  38       -5.882 -10.605   1.507  1.00  0.66           C
ATOM    251  CG1 VAL A  38       -4.841  -9.587   0.995  1.00  0.66           C
ATOM    252  CG2 VAL A  38       -5.462 -11.287   2.827  1.00  0.66
C
ATOM    253  N   GLY A  39       -7.543  -9.001   3.819  1.00  0.68           N
ATOM    254  CA  GLY A  39       -7.537  -7.952   4.844  1.00  0.68           C
ATOM    255  C   GLY A  39       -6.158  -7.700   5.397  1.00  0.68           C
ATOM    256  O   GLY A  39       -5.999  -7.288   6.540  1.00  0.68           O
ATOM    257  N   SER A  40       -5.122  -7.997   4.588  1.00  0.67           N
ATOM    258  CA  SER A  40       -3.705  -7.844   4.914  1.00  0.67           C
ATOM    259  C   SER A  40       -3.321  -6.382   5.073  1.00  0.67           C
ATOM    260  O   SER A  40       -2.645  -5.977   6.021  1.00  0.67           O
ATOM    261  CB  SER A  40       -2.815  -8.507   3.822  1.00  0.67           C
ATOM    262  OG  SER A  40       -1.435  -8.518   4.180  1.00  0.67           O
ATOM    263  N   ILE A  41       -3.815  -5.512   4.167  1.00  0.71           N
ATOM    264  CA  ILE A  41       -3.589  -4.080   4.234  1.00  0.71           C
ATOM    265  C   ILE A  41       -4.645  -3.491   5.141  1.00  0.71           C
ATOM    266  O   ILE A  41       -5.737  -3.105   4.731  1.00  0.71           O
ATOM    267  CB  ILE A  41       -3.554  -3.359   2.886  1.00  0.71           C
ATOM    268  CG1 ILE A  41       -2.420  -3.915   1.984  1.00  0.71           C
ATOM    269  CG2 ILE A  41       -3.340  -1.835   3.117  1.00  0.71           C
ATOM    270  CD1 ILE A  41       -2.741  -5.207   1.212  1.00  0.71           C
ATOM    271  N   GLY A  42       -4.319  -3.449   6.443  1.00  0.80           N
ATOM    272  CA  GLY A  42       -5.126  -2.805   7.460  1.00  0.80           C
ATOM    273  C   GLY A  42       -4.808  -1.343   7.575  1.00  0.80           C
ATOM    274  O   GLY A  42       -4.010  -0.783   6.827  1.00  0.80           O
ATOM    275  N   SER A  43       -5.388  -0.683   8.593  1.00  0.76           N
ATOM    276  CA  SER A  43       -5.141   0.722   8.903  1.00  0.76           C
ATOM    277  C   SER A  43       -3.691   1.025   9.207  1.00  0.76           C
ATOM    278  O   SER A  43       -3.152   2.046   8.773  1.00  0.76           O
ATOM    279  CB  SER A  43       -5.996   1.206  10.107  1.00  0.76           C
ATOM    280  OG  SER A  43       -5.731   0.438  11.284  1.00  0.76           O
ATOM    281  N   GLY A  44       -3.011   0.112   9.927  1.00  0.80           N
ATOM    282  CA  GLY A  44       -1.590   0.204  10.230  1.00  0.80           C
ATOM    283  C   GLY A  44       -0.724   0.082   9.013  1.00  0.80           C
ATOM    284  O   GLY A  44        0.266   0.794   8.871  1.00  0.80           O
ATOM    285  N   ILE A  45       -1.085  -0.791   8.059  1.00  0.73           N
ATOM    286  CA  ILE A  45       -0.381  -0.882   6.793  1.00  0.73           C
ATOM    287  C   ILE A  45       -0.599   0.363   5.958  1.00  0.73           C
ATOM    288  O   ILE A  45        0.378   0.924   5.480  1.00  0.73           O
ATOM    289  CB  ILE A  45       -0.735  -2.140   6.013  1.00  0.73           C
ATOM    290  CG1 ILE A  45       -0.477  -3.418   6.854  1.00  0.73           C
ATOM    291  CG2 ILE A  45        0.041  -2.198   4.673  1.00  0.73           C
ATOM    292  CD1 ILE A  45        0.979  -3.616   7.304  1.00  0.73           C
ATOM    293  N   ALA A  46       -1.855   0.859   5.832  1.00  0.80           N
ATOM    294  CA  ALA A  46       -2.228   2.062   5.101  1.00  0.80           C
ATOM    295  C   ALA A  46       -1.597   3.364   5.593  1.00  0.80           C
ATOM    296  O   ALA A  46       -1.137   4.182   4.812  1.00  0.80           O
ATOM    297  CB  ALA A  46       -3.748   2.270   5.131  1.00  0.80           C
ATOM    298  N   ALA A  47       -1.551   3.569   6.927  1.00  0.79           N
ATOM    299  CA  ALA A  47       -0.885   4.707   7.518  1.00  0.79           C
ATOM    300  C   ALA A  47        0.618   4.648   7.318  1.00  0.79           C
ATOM    301  O   ALA A  47        1.243   5.617   6.875  1.00  0.79           O
ATOM    302  CB  ALA A  47       -1.215   4.727   9.025  1.00  0.79           C
ATOM    303  N   THR A  48        1.244   3.483   7.574  1.00  0.78           N
ATOM    304  CA  THR A  48        2.681   3.298   7.401  1.00  0.78           C
ATOM    305  C   THR A  48        3.103   3.454   5.967  1.00  0.78           C
ATOM    306  O   THR A  48        4.037   4.181   5.655  1.00  0.78           O
ATOM    307  CB  THR A  48        3.159   1.938   7.873  1.00  0.78           C
ATOM    308  OG1 THR A  48        2.900   1.798   9.259  1.00  0.78           O
ATOM    309  CG2 THR A  48        4.675   1.764   7.754  1.00  0.78           C
ATOM    310  N   VAL A  49        2.384   2.815   5.030  1.00  0.80           N
ATOM    311  CA  VAL A  49        2.704   2.860   3.625  1.00  0.80           C
ATOM    312  C   VAL A  49        2.613   4.250   3.012  1.00  0.80           C
ATOM    313  O   VAL A  49        3.543   4.678   2.336  1.00  0.80           O
ATOM    314  CB  VAL A  49        1.899   1.823   2.873  1.00  0.80           C
ATOM    315  CG1 VAL A  49        0.424   2.193   2.756  1.00  0.80           C
ATOM    316  CG2 VAL A  49        2.543   1.524   1.530  1.00  0.80           C
ATOM    317  N   LEU A  50        1.558   5.051   3.296  1.00  0.75           N
ATOM    318  CA  LEU A  50        1.455   6.406   2.779  1.00  0.75           C
ATOM    319  C   LEU A  50        2.543   7.295   3.351  1.00  0.75           C
ATOM    320  O   LEU A  50        3.072   8.212   2.714  1.00  0.75           O
ATOM    321  CB  LEU A  50        0.057   7.009   3.048  1.00  0.75           C
ATOM    322  CG  LEU A  50       -0.175   8.389   2.390  1.00  0.75           C
ATOM    323  CD1 LEU A  50        0.067   8.353   0.871  1.00  0.75           C
ATOM    324  CD2 LEU A  50       -1.595   8.898   2.676  1.00  0.75           C
ATOM    325  N   TYR A  51        2.942   7.020   4.600  1.00  0.71           N
ATOM    326  CA  TYR A  51        4.029   7.710   5.250  1.00  0.71           C
ATOM    327  C   TYR A  51        5.370   7.366   4.664  1.00  0.71           C
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ATOM    328  O   TYR A  51      6.197   8.262   4.536  1.00  0.71           O
ATOM    329  CB  TYR A  51      4.039   7.494   6.775  1.00  0.71           C
ATOM    330  CG  TYR A  51      2.860   8.147   7.454  1.00  0.71           C
ATOM    331  CD1 TYR A  51      1.832   8.854   6.788  1.00  0.71           C
ATOM    332  CD2 TYR A  51      2.766   7.999   8.845  1.00  0.71           C
ATOM    333  CE1 TYR A  51      0.736   9.357   7.492  1.00  0.71           C
ATOM    334  CE2 TYR A  51      1.681   8.532   9.555  1.00  0.71           C
ATOM    335  CZ  TYR A  51      0.666   9.208   8.871  1.00  0.71           C
ATOM    336  OH  TYR A  51     -0.444   9.747   9.543  1.00  0.71           O
ATOM    337  N   ILE A  52      5.612   6.091   4.291  1.00  0.72           N
ATOM    338  CA  ILE A  52      6.763   5.620   3.525  1.00  0.72           C
ATOM    339  C   ILE A  52      6.829   6.290   2.165  1.00  0.72           C
ATOM    340  O   ILE A  52      7.891   6.753   1.760  1.00  0.72           O
ATOM    341  CB  ILE A  52      6.773   4.099   3.369  1.00  0.72           C
ATOM    342  CG1 ILE A  52      6.997   3.418   4.736  1.00  0.72           C
ATOM    343  CG2 ILE A  52      7.856   3.634   2.363  1.00  0.72           C
ATOM    344  CD1 ILE A  52      6.730   1.912   4.683  1.00  0.72           C
ATOM    345  N   LEU A  53      5.680   6.421   1.463  1.00  0.74           N
ATOM    346  CA  LEU A  53      5.570   7.117   0.182  1.00  0.74           C
ATOM    347  C   LEU A  53      5.933   8.548   0.224  1.00  0.74           C
ATOM    348  O   LEU A  53      6.474   9.108  -0.725  1.00  0.74           O
ATOM    349  CB  LEU A  53      4.166   7.049  -0.471  1.00  0.74           C
ATOM    350  CG  LEU A  53      4.154   5.825  -1.378  1.00  0.74           C
ATOM    351  CD1 LEU A  53      4.430   4.518  -0.672  1.00  0.74           C
ATOM    352  CD2 LEU A  53      2.961   5.556  -2.279  1.00  0.74           C
ATOM    353  N   LYS A  54      5.597   9.180   1.336  1.00  0.72           N
ATOM    354  CA  LYS A  54      5.916  10.551   1.548  1.00  0.72           C
ATOM    355  C   LYS A  54      7.403  10.833   1.730  1.00  0.72           C
ATOM    356  O   LYS A  54      7.921  11.798   1.182  1.00  0.72           O
ATOM    357  CB  LYS A  54      5.123  11.017   2.783  1.00  0.72           C
ATOM    358  CG  LYS A  54      5.310  12.501   3.118  1.00  0.72           C
ATOM    359  CD  LYS A  54      4.863  13.444   1.984  1.00  0.72           C
ATOM    360  CE  LYS A  54      3.367  13.407   1.662  1.00  0.72           C
ATOM    361  NZ  LYS A  54      2.611  13.931   2.819  1.00  0.72           N
ATOM    362  N   LYS A  55      8.115  10.007   2.530  1.00  0.69           N
ATOM    363  CA  LYS A  55      9.534  10.218   2.783  1.00  0.69           C
ATOM    364  C   LYS A  55     10.447   9.556   1.777  1.00  0.69           C
ATOM    365  O   LYS A  55     11.380  10.170   1.270  1.00  0.69           O
ATOM    366  CB  LYS A  55      9.968   9.768   4.214  1.00  0.69           C
ATOM    367  CG  LYS A  55      9.386   8.432   4.712  1.00  0.69           C
ATOM    368  CD  LYS A  55      9.691   8.090   6.183  1.00  0.69           C
ATOM    369  CE  LYS A  55      9.109   9.079   7.206  1.00  0.69           C
ATOM    370  NZ  LYS A  55      7.627   9.075   7.161  1.00  0.69           N
ATOM    371  N   LYS A  56     10.223   8.269   1.485  1.00  0.68           N
ATOM    372  CA  LYS A  56     11.139   7.494   0.692  1.00  0.68           C
ATOM    373  C   LYS A  56     10.633   7.310  -0.727  1.00  0.68           C
ATOM    374  O   LYS A  56     11.413   7.284  -1.675  1.00  0.68           O
ATOM    375  CB  LYS A  56     11.278   6.108   1.348  1.00  0.68           C
ATOM    376  CG  LYS A  56     11.985   6.125   2.719  1.00  0.68           C
ATOM    377  CD  LYS A  56     12.084   4.706   3.309  1.00  0.68           C
ATOM    378  CE  LYS A  56     12.877   4.537   4.611  1.00  0.68           C
ATOM    379  NZ  LYS A  56     12.877   3.120   5.078  1.00  0.68           N
ATOM    380  N   GLY A  57      9.300   7.197  -0.906  1.00  0.79           N
ATOM    381  CA  GLY A  57      8.677   7.161  -2.222  1.00  0.79           C
ATOM    382  C   GLY A  57      7.874   5.920  -2.520  1.00  0.79           C
ATOM    383  O   GLY A  57      7.926   4.903  -1.821  1.00  0.79           O
ATOM    384  N   ALA A  58      7.097   5.978  -3.620  1.00  0.80           N
ATOM    385  CA  ALA A  58      6.190   4.944  -4.096  1.00  0.80           C
ATOM    386  C   ALA A  58      6.826   3.604  -4.378  1.00  0.80           C
ATOM    387  O   ALA A  58      6.342   2.550  -3.964  1.00  0.80           O
ATOM    388  CB  ALA A  58      5.426   5.513  -5.308  1.00  0.80           C
ATOM    389  N   ALA A  59      7.990   3.627  -5.022  1.00  0.77           N
ATOM    390  CA  ALA A  59      8.762   2.448  -5.289  1.00  0.77           C
ATOM    391  C   ALA A  59      9.342   1.818  -4.030  1.00  0.77           C
ATOM    392  O   ALA A  59      9.486   0.594  -3.934  1.00  0.77           O
ATOM    393  CB  ALA A  59      9.853   2.866  -6.280  1.00  0.77           C
ATOM    394  N   LYS A  60      9.670   2.621  -2.999  1.00  0.71           N
ATOM    395  CA  LYS A  60     10.187   2.089  -1.761  1.00  0.71           C
ATOM    396  C   LYS A  60      9.185   1.267  -0.994  1.00  0.71           C
ATOM    397  O   LYS A  60      9.487   0.199  -0.471  1.00  0.71           O
ATOM    398  CB  LYS A  60     10.604   3.198  -0.782  1.00  0.71           C
ATOM    399  CG  LYS A  60     11.137   2.640   0.553  1.00  0.71           C
ATOM    400  CD  LYS A  60     12.485   1.918   0.383  1.00  0.71           C
ATOM    401  CE  LYS A  60     13.134   1.463   1.690  1.00  0.71           C
ATOM    402  NZ  LYS A  60     14.401   0.735   1.439  1.00  0.71           N
ATOM    403  N   ALA A  61      7.955   1.780  -0.876  1.00  0.80           N
ATOM    404  CA  ALA A  61      6.961   1.014  -0.188  1.00  0.80           C
ATOM    405  C   ALA A  61      6.417  -0.074  -1.034  1.00  0.80           C
ATOM    406  O   ALA A  61      5.898  -1.062  -0.443  1.00  0.80           O
ATOM    407  CB  ALA A  61      5.747   1.837   0.097  1.00  0.80           C
ATOM    408  N   ALA A  62      6.503  -0.065  -2.351  1.00  0.80           N
ATOM    409  CA  ALA A  62      6.152  -1.200  -3.159  1.00  0.80           C
ATOM    410  C   ALA A  62      6.983  -2.415  -2.717  1.00  0.80           C
ATOM    411  O   ALA A  62      6.445  -3.489  -2.429  1.00  0.80           O
ATOM    412  CB  ALA A  62      6.384  -0.873  -4.645  1.00  0.80           C
ATOM    413  N   LEU A  63      8.298  -2.191  -2.521  1.00  0.65           N
ATOM    414  CA  LEU A  63      9.246  -3.154  -1.982  1.00  0.65           C
ATOM    415  C   LEU A  63      9.161  -3.576  -0.513  1.00  0.65           C
ATOM    416  O   LEU A  63      9.526  -4.705  -0.225  1.00  0.65           O
ATOM    417  CB  LEU A  63     10.702  -2.673  -2.121  1.00  0.65           C
ATOM    418  CG  LEU A  63     11.239  -2.545  -3.550  1.00  0.65           C
ATOM    419  CD1 LEU A  63     12.637  -1.915  -3.469  1.00  0.65
C
ATOM    420  CD2 LEU A  63     11.307  -3.913  -4.251  1.00  0.65
C
ATOM    421  N   TRP A  64      8.758  -2.647   0.405  1.00  0.64           N
ATOM    422  CA  TRP A  64      8.711  -2.768   1.865  1.00  0.64           C
ATOM    423  C   TRP A  64      7.821  -3.938   2.334  1.00  0.64           C
ATOM    424  O   TRP A  64      7.686  -4.945   1.627  1.00  0.64           O
ATOM    425  CB  TRP A  64      8.147  -1.426   2.467  1.00  0.64           C
ATOM    426  CG  TRP A  64      7.687  -1.325   3.941  1.00  0.64           C
ATOM    427  CD1 TRP A  64      8.484  -1.476   5.033  1.00  0.64           C
ATOM    428  CD2 TRP A  64      6.318  -1.341   4.449  1.00  0.64           C
ATOM    429  NE1 TRP A  64      7.733  -1.546   6.187  1.00  0.64           N
ATOM    430  CE2 TRP A  64      6.402  -1.504   5.848  1.00  0.64           C
ATOM    431  CE3 TRP A  64      5.065  -1.266   3.827  1.00  0.64           C
ATOM    432  CZ2 TRP A  64      5.261  -1.624   6.635  1.00  0.64           C
ATOM    433  CZ3 TRP A  64      3.914  -1.365   4.629  1.00  0.64           C
ATOM    434  CH2 TRP A  64      4.009  -1.552   6.011  1.00  0.64           C
ATOM    435  OXT TRP A  64      7.076  -3.793   3.329  1.00  0.64           O
TER     436      TRP A  64
END
```

B)

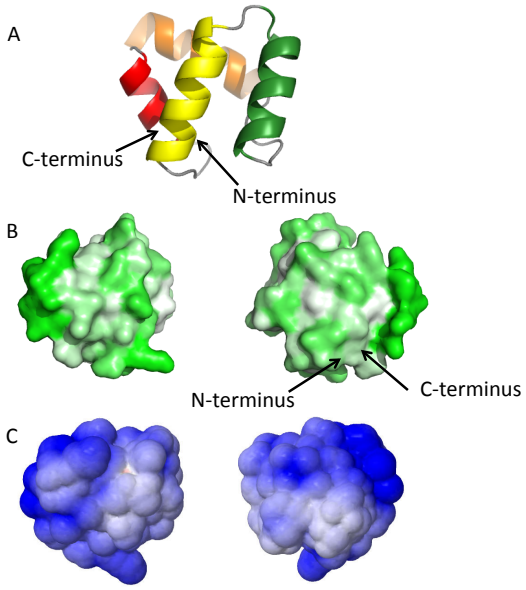

Figure S1- Structural models of pneumocyclicin. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of pneumocyclicin. Orientation peptide backbone in surface filling diagrams, B and C, correlate to one another.

2. Aureocyclicin

A) PDB file for model of aureocyclicin. Structure modeled after NKR-5-3B using SWISS-MODEL.[84]

TITLE SWISS-MODEL SERVER (https://swissmodel.expasy.org)
TITLE 2 Untitled Project
EXPDTA THEORETICAL MODEL (SWISS-MODEL SERVER)
AUTHOR SWISS-MODEL SERVER (SEE REFERENCE IN JRNL Records)
REVDAT 1 31-OCT-16 1MOD 1 15:49
JRNL AUTH
M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO
CASSARINO,M.BERTONI,L.BORDOLI,
JRNL AUTH 3 T.SCHWEDE
JRNL TITL SWISS-MODEL: MODELLING PROTEIN TERTIARY AND QUATERNARY
JRNL TITL 2 STRUCTURE USING EVOLUTIONARY INFORMATION
JRNL REF NUCLEIC.ACIDS.RES 2014
JRNL REFN ISSN 0305-1048
JRNL PMID 24782522
JRNL DOI 10.1093/nar/gku340
REMARK 3 MODEL INFORMATION
REMARK 3 ENGIN PROMOD3
REMARK 3 VERSN 1.0.1
REMARK 3 OSTAT MONOMER
REMARK 3 OSRSN USER
REMARK 3 GMQE 0.68
REMARK 3 QMN4 -1.58
REMARK 3 MODT FALSE
REMARK 3
REMARK 3 TEMPLATE 1
REMARK 3 PDBID 2mp8
REMARK 3 CHAIN A
REMARK 3 MMCIF A
REMARK 3 PDBV 2016-10-14
REMARK 3 SMTLE 2mp8.1.A
REMARK 3 SMTLV 2016-10-19
REMARK 3 MTHD SOLUTION NMR 0.00 A
REMARK 3 FOUND HHblits
REMARK 3 GMQE 0.68
REMARK 3 SIM 0.38
REMARK 3 SID 36.84
REMARK 3 OSTAT monomer
ATOM 1 N LEU A 4 4.118 -7.799 3.715 1.00 0.49 N
ATOM 2 CA LEU A 4 2.872 -8.607 3.431 1.00 0.49 C
ATOM 3 C LEU A 4 2.972 -9.947 2.742 1.00 0.49 C
ATOM 4 O LEU A 4 2.131 -10.807 2.958 1.00 0.49 O
ATOM 5 CB LEU A 4 1.992 -7.724 2.568 1.00 0.49 C
ATOM 6 CG LEU A 4 1.872 -6.310 3.139 1.00 0.49 C
ATOM 7 CD1 LEU A 4 1.204 -5.517 2.071 1.00 0.49 C
ATOM 8 CD2 LEU A 4 1.086 -6.190 4.446 1.00 0.49 C
ATOM 9 N GLY A 5 3.996 -10.151 1.888 1.00 0.58 N
ATOM 10 CA GLY A 5 4.157 -11.403 1.146 1.00 0.58 C
ATOM 11 C GLY A 5 3.320 -11.453 -0.109 1.00 0.58 C
ATOM 12 O GLY A 5 2.771 -12.486 -0.469 1.00 0.58 O
ATOM 13 N ILE A 6 3.197 -10.304 -0.799 1.00 0.54 N

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ATOM     14  CA  ILE A   6       2.385 -10.148  -1.987  1.00  0.54           C
ATOM     15  C   ILE A   6       3.318  -9.942  -3.162  1.00  0.54           C
ATOM     16  O   ILE A   6       4.507  -9.684  -2.991  1.00  0.54           O
ATOM     17  CB  ILE A   6       1.405  -8.977  -1.903  1.00  0.54           C
ATOM     18  CG1 ILE A   6       2.101  -7.610  -1.685  1.00  0.54           C
ATOM     19  CG2 ILE A   6       0.360  -9.320  -0.822  1.00  0.54           C
ATOM     20  CD1 ILE A   6       1.140  -6.425  -1.804  1.00  0.54           C
ATOM     21  N   GLY A   7       2.809 -10.075  -4.405  1.00  0.70           N
ATOM     22  CA  GLY A   7       3.583  -9.762  -5.604  1.00  0.70           C
ATOM     23  C   GLY A   7       3.844  -8.281  -5.799  1.00  0.70           C
ATOM     24  O   GLY A   7       3.115  -7.432  -5.298  1.00  0.70           O
ATOM     25  N   THR A   8       4.851  -7.928  -6.622  1.00  0.64           N
ATOM     26  CA  THR A   8       5.173  -6.552  -7.002  1.00  0.64           C
ATOM     27  C   THR A   8       4.046  -5.864  -7.749  1.00  0.64           C
ATOM     28  O   THR A   8       3.789  -4.679  -7.567  1.00  0.64           O
ATOM     29  CB  THR A   8       6.436  -6.457  -7.847  1.00  0.64           C
ATOM     30  OG1 THR A   8       6.383  -7.315  -8.984  1.00  0.64           O
ATOM     31  CG2 THR A   8       7.624  -6.924  -6.998  1.00  0.64           C
ATOM     32  N   GLY A   9       3.339  -6.627  -8.612  1.00  0.73           N
ATOM     33  CA  GLY A   9       2.092  -6.245  -9.272  1.00  0.73           C
ATOM     34  C   GLY A   9       0.999  -5.821  -8.337  1.00  0.73           C
ATOM     35  O   GLY A   9       0.437  -4.740  -8.468  1.00  0.73           O
ATOM     36  N   MET A  10       0.682  -6.663  -7.328  1.00  0.65           N
ATOM     37  CA  MET A  10      -0.220  -6.273  -6.264  1.00  0.65           C
ATOM     38  C   MET A  10       0.311  -5.066  -5.517  1.00  0.65           C
ATOM     39  O   MET A  10      -0.381  -4.066  -5.429  1.00  0.65           O
ATOM     40  CB  MET A  10      -0.471  -7.419  -5.263  1.00  0.65           C
ATOM     41  CG  MET A  10      -1.242  -8.607  -5.861  1.00  0.65           C
ATOM     42  SD  MET A  10      -1.285 -10.058  -4.766  1.00  0.65           S
ATOM     43  CE  MET A  10      -2.453  -9.332  -3.584  1.00  0.65           C
ATOM     44  N   ALA A  11       1.584  -5.076  -5.072  1.00  0.73           N
ATOM     45  CA  ALA A  11       2.165  -3.953  -4.365  1.00  0.73           C
ATOM     46  C   ALA A  11       2.070  -2.612  -5.114  1.00  0.73           C
ATOM     47  O   ALA A  11       1.596  -1.625  -4.574  1.00  0.73           O
ATOM     48  CB  ALA A  11       3.627  -4.276  -4.022  1.00  0.73           C
ATOM     49  N   ALA A  12       2.408  -2.549  -6.412  1.00  0.75           N
ATOM     50  CA  ALA A  12       2.209  -1.371  -7.244  1.00  0.75           C
ATOM     51  C   ALA A  12       0.763  -0.905  -7.406  1.00  0.75           C
ATOM     52  O   ALA A  12       0.451   0.286  -7.411  1.00  0.75           O
ATOM     53  CB  ALA A  12       2.773  -1.667  -8.637  1.00  0.75           C
ATOM     54  N   THR A  13      -0.173  -1.856  -7.527  1.00  0.74           N
ATOM     55  CA  THR A  13      -1.603  -1.590  -7.516  1.00  0.74           C
ATOM     56  C   THR A  13      -2.084  -0.990  -6.218  1.00  0.74           C
ATOM     57  O   THR A  13      -2.882  -0.051  -6.181  1.00  0.74           O
ATOM     58  CB  THR A  13      -2.394  -2.849  -7.748  1.00  0.74           C
ATOM     59  OG1 THR A  13      -2.185  -3.329  -9.065  1.00  0.74           O
ATOM     60  CG2 THR A  13      -3.876  -2.534  -7.668  1.00  0.74           C
ATOM     61  N   ILE A  14      -1.576  -1.516  -5.099  1.00  0.73           N
ATOM     62  CA  ILE A  14      -1.814  -0.951  -3.797  1.00  0.73           C
ATOM     63  C   ILE A  14      -1.330   0.493  -3.692  1.00  0.73           C
ATOM     64  O   ILE A  14      -2.054   1.377  -3.238  1.00  0.73           O
ATOM     65  CB  ILE A  14      -1.045  -1.701  -2.747  1.00  0.73           C
ATOM     66  CG1 ILE A  14      -1.377  -3.201  -2.560  1.00  0.73           C
ATOM     67  CG2 ILE A  14      -1.234  -0.935  -1.445  1.00  0.73           C
ATOM     68  CD1 ILE A  14      -2.747  -3.509  -1.981  1.00  0.73           C
ATOM     69  N   ILE A  15      -0.087   0.768  -4.147  1.00  0.71           N
ATOM     70  CA  ILE A  15       0.518   2.092  -4.156  1.00  0.71           C
ATOM     71  C   ILE A  15      -0.336   3.105  -4.852  1.00  0.71           C
ATOM     72  O   ILE A  15      -0.457   4.245  -4.407  1.00  0.71           O
ATOM     73  CB  ILE A  15       1.817   2.085  -4.917  1.00  0.71           C
ATOM     74  CG1 ILE A  15       2.913   1.305  -4.204  1.00  0.71           C
ATOM     75  CG2 ILE A  15       2.348   3.464  -5.371  1.00  0.71           C
ATOM     76  CD1 ILE A  15       3.286   1.653  -2.771  1.00  0.71           C
ATOM     77  N   ASN A  16      -0.959   2.710  -5.976  1.00  0.74           N
ATOM     78  CA  ASN A  16      -1.916   3.565  -6.635  1.00  0.74           C
ATOM     79  C   ASN A  16      -3.065   3.960  -5.716  1.00  0.74           C
ATOM     80  O   ASN A  16      -3.348   5.134  -5.529  1.00  0.74           O
ATOM     81  CB  ASN A  16      -2.467   2.888  -7.905  1.00  0.74           C
ATOM     82  CG  ASN A  16      -1.362   2.856  -8.955  1.00  0.74           C
ATOM     83  OD1 ASN A  16      -0.448   3.683  -8.966  1.00  0.74           O
ATOM     84  ND2 ASN A  16      -1.467   1.897  -9.901  1.00  0.74           N
ATOM     85  N   ALA A  17      -3.691   2.988  -5.046  1.00  0.77           N
ATOM     86  CA  ALA A  17      -4.770   3.208  -4.122  1.00  0.77           C
ATOM     87  C   ALA A  17      -4.468   3.986  -2.838  1.00  0.77           C
ATOM     88  O   ALA A  17      -5.254   4.845  -2.447  1.00  0.77           O
ATOM     89  CB  ALA A  17      -5.375   1.830  -3.852  1.00  0.77           C
ATOM     90  N   ILE A  18      -3.323   3.731  -2.165  1.00  0.70           N
ATOM     91  CA  ILE A  18      -2.878   4.501  -0.996  1.00  0.70           C
ATOM     92  C   ILE A  18      -2.452   5.922  -1.332  1.00  0.70           C
ATOM     93  O   ILE A  18      -2.525   6.820  -0.496  1.00  0.70           O
ATOM     94  CB  ILE A  18      -1.738   3.864  -0.191  1.00  0.70           C
ATOM     95  CG1 ILE A  18      -0.446   3.710  -1.015  1.00  0.70           C
ATOM     96  CG2 ILE A  18      -2.181   2.504   0.363  1.00  0.70           C
ATOM     97  CD1 ILE A  18       0.744   3.136  -0.248  1.00  0.70           C
ATOM     98  N   SER A  19      -1.945   6.120  -2.566  1.00  0.72           N
ATOM     99  CA  SER A  19      -1.619   7.417  -3.141  1.00  0.72           C
ATOM    100  C   SER A  19      -2.824   8.231  -3.581  1.00  0.72           C
ATOM    101  O   SER A  19      -2.831   9.449  -3.457  1.00  0.72           O
ATOM    102  CB  SER A  19      -0.777   7.277  -4.442  1.00  0.72           C
ATOM    103  OG  SER A  19       0.523   6.709  -4.255  1.00  0.72           O
ATOM    104  N   VAL A  20      -3.837   7.582  -4.190  1.00  0.63           N
ATOM    105  CA  VAL A  20      -5.060   8.228  -4.666  1.00  0.63           C
ATOM    106  C   VAL A  20      -6.043   8.490  -3.539  1.00  0.63           C
ATOM    107  O   VAL A  20      -6.636   9.562  -3.420  1.00  0.63           O
ATOM    108  CB  VAL A  20      -5.749   7.390  -5.753  1.00  0.63           C
ATOM    109  CG1 VAL A  20      -7.114   7.977  -6.165  1.00  0.63           C
ATOM    110  CG2 VAL A  20      -4.862   7.367  -7.012  1.00  0.63           C
ATOM    111  N   GLY A  21      -6.269   7.485  -2.672  1.00  0.68           N
ATOM    112  CA  GLY A  21      -7.202   7.605  -1.570  1.00  0.68           C
ATOM    113  C   GLY A  21      -6.700   8.483  -0.444  1.00  0.68           C
ATOM    114  O   GLY A  21      -5.519   8.533  -0.117  1.00  0.68           O
ATOM    115  N   LEU A  22      -7.627   9.177   0.239  1.00  0.51           N
ATOM    116  CA  LEU A  22      -7.282  10.136   1.272  1.00  0.51           C
ATOM    117  C   LEU A  22      -7.477   9.541   2.657  1.00  0.51           C
ATOM    118  O   LEU A  22      -6.519   9.218   3.364  1.00  0.51           O
ATOM    119  CB  LEU A  22      -8.162  11.402   1.142  1.00  0.51           C
ATOM    120  CG  LEU A  22      -7.900  12.224  -0.132  1.00  0.51           C
ATOM    121  CD1 LEU A  22      -8.936  13.354  -0.221  1.00  0.51
C
ATOM    122  CD2 LEU A  22      -6.469  12.781  -0.187  1.00  0.51
C
ATOM    123  N   SER A  23      -8.752   9.391   3.073  1.00  0.59           N
ATOM    124  CA  SER A  23      -9.172   8.796   4.341  1.00  0.59           C
ATOM    125  C   SER A  23      -8.710   7.347   4.472  1.00  0.59           C
ATOM    126  O   SER A  23      -8.851   6.556   3.544  1.00  0.59           O
ATOM    127  CB  SER A  23     -10.720   8.839   4.505  1.00  0.59           C
ATOM    128  OG  SER A  23     -11.167   8.248   5.729  1.00  0.59           O
ATOM    129  N   ALA A  24      -8.155   6.952   5.638  1.00  0.70           N
ATOM    130  CA  ALA A  24      -7.600   5.631   5.863  1.00  0.70           C
ATOM    131  C   ALA A  24      -8.601   4.486   5.716  1.00  0.70           C
ATOM    132  O   ALA A  24      -8.313   3.470   5.093  1.00  0.70           O
ATOM    133  CB  ALA A  24      -6.973   5.608   7.268  1.00  0.70           C
ATOM    134  N   ALA A  25      -9.828   4.657   6.245  1.00  0.72           N
ATOM    135  CA  ALA A  25     -10.919   3.709   6.114  1.00  0.72           C
ATOM    136  C   ALA A  25     -11.326   3.485   4.659  1.00  0.72           C
ATOM    137  O   ALA A  25     -11.548   2.359   4.218  1.00  0.72           O
ATOM    138  CB  ALA A  25     -12.126   4.222   6.925  1.00  0.72           C
ATOM    139  N   THR A  26     -11.379   4.581   3.867  1.00  0.68           N
ATOM    140  CA  THR A  26     -11.651   4.550   2.428  1.00  0.68           C
ATOM    141  C   THR A  26     -10.598   3.768   1.672  1.00  0.68           C
ATOM    142  O   THR A  26     -10.906   2.894   0.866  1.00  0.68           O
ATOM    143  CB  THR A  26     -11.725   5.949   1.811  1.00  0.68           C
ATOM    144  OG1 THR A  26     -12.708   6.738   2.467  1.00  0.68
O
ATOM    145  CG2 THR A  26     -12.120   5.936   0.327  1.00  0.68
C
ATOM    146  N   ILE A  27      -9.304   4.025   1.961  1.00  0.67           N
ATOM    147  CA  ILE A  27      -8.198   3.291   1.373  1.00  0.67           C
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ATOM    148  C   ILE A  27      -8.231   1.812   1.771  1.00  0.67           C
ATOM    149  O   ILE A  27      -8.084   0.949   0.916  1.00  0.67           O
ATOM    150  CB  ILE A  27      -6.833   3.904   1.695  1.00  0.67           C
ATOM    151  CG1 ILE A  27      -6.705   5.399   1.350  1.00  0.67           C
ATOM    152  CG2 ILE A  27      -5.745   3.202   0.873  1.00  0.67           C
ATOM    153  CD1 ILE A  27      -5.533   6.083   2.066  1.00  0.67           C
ATOM    154  N   LEU A  28      -8.501   1.461   3.053  1.00  0.72           N
ATOM    155  CA  LEU A  28      -8.553   0.065   3.507  1.00  0.72           C
ATOM    156  C   LEU A  28      -9.498  -0.809   2.705  1.00  0.72           C
ATOM    157  O   LEU A  28      -9.149  -1.892   2.242  1.00  0.72           O
ATOM    158  CB  LEU A  28      -9.081  -0.034   4.959  1.00  0.72           C
ATOM    159  CG  LEU A  28      -8.994  -1.432   5.617  1.00  0.72           C
ATOM    160  CD1 LEU A  28      -7.615  -2.109   5.539  1.00  0.72           C
ATOM    161  CD2 LEU A  28      -9.469  -1.337   7.072  1.00  0.72           C
ATOM    162  N   SER A  29     -10.723  -0.294   2.509  1.00  0.79           N
ATOM    163  CA  SER A  29     -11.780  -0.887   1.711  1.00  0.79           C
ATOM    164  C   SER A  29     -11.454  -1.055   0.240  1.00  0.79           C
ATOM    165  O   SER A  29     -11.790  -2.062  -0.375  1.00  0.79           O
ATOM    166  CB  SER A  29     -13.068  -0.045   1.803  1.00  0.79           C
ATOM    167  OG  SER A  29     -13.572  -0.046   3.140  1.00  0.79           O
ATOM    168  N   LEU A  30     -10.793  -0.061  -0.386  1.00  0.73           N
ATOM    169  CA  LEU A  30     -10.335  -0.189  -1.760  1.00  0.73           C
ATOM    170  C   LEU A  30      -9.206  -1.179  -1.910  1.00  0.73           C
ATOM    171  O   LEU A  30      -9.209  -2.041  -2.784  1.00  0.73           O
ATOM    172  CB  LEU A  30      -9.866   1.164  -2.327  1.00  0.73           C
ATOM    173  CG  LEU A  30     -10.981   2.220  -2.380  1.00  0.73           C
ATOM    174  CD1 LEU A  30     -10.411   3.556  -2.870  1.00  0.73
C
ATOM    175  CD2 LEU A  30     -12.202   1.776  -3.203  1.00  0.73
C
ATOM    176  N   ILE A  31      -8.218  -1.107  -1.010  1.00  0.71           N
ATOM    177  CA  ILE A  31      -7.112  -2.045  -0.983  1.00  0.71           C
ATOM    178  C   ILE A  31      -7.556  -3.483  -0.780  1.00  0.71           C
ATOM    179  O   ILE A  31      -7.117  -4.403  -1.475  1.00  0.71           O
ATOM    180  CB  ILE A  31      -6.154  -1.693   0.132  1.00  0.71           C
ATOM    181  CG1 ILE A  31      -5.413  -0.368  -0.065  1.00  0.71           C
ATOM    182  CG2 ILE A  31      -5.143  -2.826   0.333  1.00  0.71           C
ATOM    183  CD1 ILE A  31      -4.679  -0.354  -1.388  1.00  0.71           C
ATOM    184  N   SER A  32      -8.463  -3.716   0.179  1.00  0.77           N
ATOM    185  CA  SER A  32      -8.951  -5.043   0.483  1.00  0.77           C
ATOM    186  C   SER A  32      -9.691  -5.696  -0.666  1.00  0.77           C
ATOM    187  O   SER A  32      -9.499  -6.880  -0.942  1.00  0.77           O
ATOM    188  CB  SER A  32      -9.793  -5.064   1.784  1.00  0.77           C
ATOM    189  OG  SER A  32     -11.033  -4.375   1.640  1.00  0.77           O
ATOM    190  N   GLY A  33     -10.501  -4.890  -1.385  1.00  0.76           N
ATOM    191  CA  GLY A  33     -11.214  -5.274  -2.596  1.00  0.76
C
ATOM    192  C   GLY A  33     -10.350  -5.622  -3.781  1.00  0.76           C
ATOM    193  O   GLY A  33     -10.717  -6.446  -4.610  1.00  0.76           O
ATOM    194  N   VAL A  34      -9.174  -4.987  -3.898  1.00  0.71           N
ATOM    195  CA  VAL A  34      -8.213  -5.277  -4.944  1.00  0.71           C
ATOM    196  C   VAL A  34      -7.286  -6.456  -4.651  1.00  0.71           C
ATOM    197  O   VAL A  34      -7.078  -7.334  -5.485  1.00  0.71           O
ATOM    198  CB  VAL A  34      -7.358  -4.049  -5.154  1.00  0.71           C
ATOM    199  CG1 VAL A  34      -6.233  -4.343  -6.144  1.00  0.71
C
ATOM    200  CG2 VAL A  34      -8.187  -2.906  -5.763  1.00  0.71
C
ATOM    201  N   ALA A  35      -6.667  -6.504  -3.451  1.00  0.73           N
ATOM    202  CA  ALA A  35      -5.713  -7.544  -3.108  1.00  0.73           C
ATOM    203  C   ALA A  35      -6.373  -8.851  -2.667  1.00  0.73           C
ATOM    204  O   ALA A  35      -5.713  -9.875  -2.521  1.00  0.73           O
ATOM    205  CB  ALA A  35      -4.765  -7.053  -1.993  1.00  0.73           C
ATOM    206  N   SER A  36      -7.701  -8.819  -2.426  1.00  0.60           N
ATOM    207  CA  SER A  36      -8.521  -9.954  -2.014  1.00  0.60           C
ATOM    208  C   SER A  36      -8.133 -10.504  -0.655  1.00  0.60           C
ATOM    209  O   SER A  36      -8.057 -11.705  -0.418  1.00  0.60           O
ATOM    210  CB  SER A  36      -8.662 -11.081  -3.069  1.00  0.60           C
ATOM    211  OG  SER A  36      -9.266 -10.587  -4.270  1.00  0.60           O
ATOM    212  N   GLY A  37      -7.901  -9.597   0.311  1.00  0.61           N
ATOM    213  CA  GLY A  37      -7.475 -10.018   1.637  1.00  0.61           C
ATOM    214  C   GLY A  37      -7.354  -8.877   2.595  1.00  0.61           C
ATOM    215  O   GLY A  37      -7.553  -9.034   3.791  1.00  0.61           O
ATOM    216  N   GLY A  38      -7.015  -7.662   2.106  1.00  0.69           N
ATOM    217  CA  GLY A  38      -6.928  -6.482   2.973  1.00  0.69           C
ATOM    218  C   GLY A  38      -5.725  -6.473   3.853  1.00  0.69           C
ATOM    219  O   GLY A  38      -5.593  -5.664   4.764  1.00  0.69           O
ATOM    220  N   ALA A  39      -4.793  -7.387   3.559  1.00  0.65           N
ATOM    221  CA  ALA A  39      -3.497  -7.447   4.168  1.00  0.65           C
ATOM    222  C   ALA A  39      -2.645  -6.339   3.588  1.00  0.65           C
ATOM    223  O   ALA A  39      -1.895  -6.544   2.628  1.00  0.65           O
ATOM    224  CB  ALA A  39      -2.892  -8.858   4.003  1.00  0.65           C
ATOM    225  N   TRP A  40      -2.801  -5.112   4.113  1.00  0.68           N
ATOM    226  CA  TRP A  40      -2.002  -3.974   3.732  1.00  0.68           C
ATOM    227  C   TRP A  40      -1.921  -2.976   4.880  1.00  0.68           C
ATOM    228  O   TRP A  40      -2.880  -2.749   5.614  1.00  0.68           O
ATOM    229  CB  TRP A  40      -2.506  -3.277   2.443  1.00  0.68           C
ATOM    230  CG  TRP A  40      -1.622  -2.121   2.018  1.00  0.68           C
ATOM    231  CD1 TRP A  40      -1.788  -0.792   2.298  1.00  0.68           C
ATOM    232  CD2 TRP A  40      -0.386  -2.225   1.325  1.00  0.68           C
ATOM    233  NE1 TRP A  40      -0.671  -0.091   1.927  1.00  0.68           N
ATOM    234  CE2 TRP A  40       0.209  -0.940   1.338  1.00  0.68           C
ATOM    235  CE3 TRP A  40       0.193  -3.242   0.574  1.00  0.68           C
ATOM    236  CZ2 TRP A  40       1.415  -0.711   0.704  1.00  0.68           C
ATOM    237  CZ3 TRP A  40       1.378  -2.980  -0.133  1.00  0.68           C
ATOM    238  CH2 TRP A  40       2.001  -1.735  -0.053  1.00  0.68           C
ATOM    239  N   VAL A  41      -0.751  -2.326   5.034  1.00  0.76           N
ATOM    240  CA  VAL A  41      -0.508  -1.298   6.036  1.00  0.76           C
ATOM    241  C   VAL A  41      -0.789   0.088   5.482  1.00  0.76           C
ATOM    242  O   VAL A  41      -0.023   0.632   4.706  1.00  0.76           O
ATOM    243  CB  VAL A  41       0.960  -1.257   6.442  1.00  0.76           C
ATOM    244  CG1 VAL A  41       1.253  -0.021   7.330  1.00  0.76           C
ATOM    245  CG2 VAL A  41       1.304  -2.555   7.186  1.00  0.76           C
ATOM    246  N   LEU A  42      -1.869   0.770   5.885  1.00  0.72           N
ATOM    247  CA  LEU A  42      -2.168   2.024   5.220  1.00  0.72           C
ATOM    248  C   LEU A  42      -1.383   3.255   5.608  1.00  0.72           C
ATOM    249  O   LEU A  42      -0.790   3.945   4.782  1.00  0.72           O
ATOM    250  CB  LEU A  42      -3.596   2.354   5.600  1.00  0.72           C
ATOM    251  CG  LEU A  42      -4.567   1.315   5.072  1.00  0.72           C
ATOM    252  CD1 LEU A  42      -5.897   1.636   5.711  1.00  0.72           C
ATOM    253  CD2 LEU A  42      -4.695   1.459   3.561  1.00  0.72           C
ATOM    254  N   ALA A  43      -1.403   3.547   6.918  1.00  0.78           N
ATOM    255  CA  ALA A  43      -0.800   4.702   7.535  1.00  0.78           C
ATOM    256  C   ALA A  43       0.712   4.707   7.367  1.00  0.78           C
ATOM    257  O   ALA A  43       1.315   5.716   7.016  1.00  0.78           O
ATOM    258  CB  ALA A  43      -1.210   4.718   9.021  1.00  0.78           C
ATOM    259  N   GLY A  44       1.341   3.528   7.552  1.00  0.82           N
ATOM    260  CA  GLY A  44       2.772   3.343   7.357  1.00  0.82           C
ATOM    261  C   GLY A  44       3.212   3.373   5.912  1.00  0.82           C
ATOM    262  O   GLY A  44       4.246   3.944   5.590  1.00  0.82           O
ATOM    263  N   ALA A  45       2.435   2.780   4.981  1.00  0.79           N
ATOM    264  CA  ALA A  45       2.753   2.863   3.574  1.00  0.79           C
ATOM    265  C   ALA A  45       2.650   4.273   3.007  1.00  0.79           C
ATOM    266  O   ALA A  45       3.576   4.748   2.361  1.00  0.79           O
ATOM    267  CB  ALA A  45       1.851   1.913   2.790  1.00  0.79           C
ATOM    268  N   LYS A  46       1.565   5.032   3.287  1.00  0.74           N
ATOM    269  CA  LYS A  46       1.465   6.409   2.821  1.00  0.74           C
ATOM    270  C   LYS A  46       2.548   7.342   3.374  1.00  0.74           C
ATOM    271  O   LYS A  46       3.019   8.252   2.694  1.00  0.74           O
ATOM    272  CB  LYS A  46       0.054   7.023   3.003  1.00  0.74           C
ATOM    273  CG  LYS A  46      -0.377   7.320   4.446  1.00  0.74           C
ATOM    274  CD  LYS A  46      -1.561   8.300   4.508  1.00  0.74           C
ATOM    275  CE  LYS A  46      -2.854   7.778   3.874  1.00  0.74           C
ATOM    276  NZ  LYS A  46      -3.837   8.876   3.776  1.00  0.74           N
ATOM    277  N   GLN A  47       2.971   7.118   4.637  1.00  0.74           N
ATOM    278  CA  GLN A  47       4.105   7.783   5.254  1.00  0.74           C
ATOM    279  C   GLN A  47       5.442   7.415   4.610  1.00  0.74           C
ATOM    280  O   GLN A  47       6.256   8.277   4.286  1.00  0.74           O
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ATOM    281  CB  GLN A  47       4.127   7.493   6.774  1.00  0.74           C
ATOM    282  CG  GLN A  47       5.126   8.355   7.579  1.00  0.74           C
ATOM    283  CD  GLN A  47       4.814   9.843   7.414  1.00  0.74           C
ATOM    284  OE1 GLN A  47       3.660  10.277   7.469  1.00  0.74
O
ATOM    285  NE2 GLN A  47       5.862  10.665   7.187  1.00  0.74
N
ATOM    286  N   ALA A  48       5.666   6.113   4.320  1.00  0.81           N
ATOM    287  CA  ALA A  48       6.814   5.628   3.568  1.00  0.81           C
ATOM    288  C   ALA A  48       6.899   6.227   2.168  1.00  0.81           C
ATOM    289  O   ALA A  48       7.963   6.580   1.664  1.00  0.81           O
ATOM    290  CB  ALA A  48       6.771   4.088   3.465  1.00  0.81           C
ATOM    291  N   LEU A  49       5.744   6.388   1.516  1.00  0.74           N
ATOM    292  CA  LEU A  49       5.593   7.077   0.252  1.00  0.74           C
ATOM    293  C   LEU A  49       5.887   8.542   0.254  1.00  0.74           C
ATOM    294  O   LEU A  49       6.332   9.107  -0.742  1.00  0.74           O
ATOM    295  CB  LEU A  49       4.188   6.863  -0.292  1.00  0.74           C
ATOM    296  CG  LEU A  49       4.196   5.547  -1.081  1.00  0.74           C
ATOM    297  CD1 LEU A  49       4.631   4.221  -0.421  1.00  0.74           C
ATOM    298  CD2 LEU A  49       2.915   5.398  -1.872  1.00  0.74           C
ATOM    299  N   LYS A  50       5.589   9.194   1.372  1.00  0.77           N
ATOM    300  CA  LYS A  50       5.925  10.566   1.580  1.00  0.77           C
ATOM    301  C   LYS A  50       7.420  10.835   1.754  1.00  0.77           C
ATOM    302  O   LYS A  50       7.946  11.785   1.183  1.00  0.77           O
ATOM    303  CB  LYS A  50       5.131  11.038   2.810  1.00  0.77           C
ATOM    304  CG  LYS A  50       5.307  12.524   3.128  1.00  0.77           C
ATOM    305  CD  LYS A  50       4.861  13.463   1.995  1.00  0.77           C
ATOM    306  CE  LYS A  50       3.373  13.424   1.660  1.00  0.77           C
ATOM    307  NZ  LYS A  50       2.632  13.923   2.831  1.00  0.77           N
ATOM    308  N   GLU A  51       8.126  10.016   2.560  1.00  0.75           N
ATOM    309  CA  GLU A  51       9.550  10.196   2.802  1.00  0.75           C
ATOM    310  C   GLU A  51      10.480   9.509   1.807  1.00  0.75           C
ATOM    311  O   GLU A  51      11.404  10.119   1.275  1.00  0.75           O
ATOM    312  CB  GLU A  51       9.888   9.699   4.220  1.00  0.75           C
ATOM    313  CG  GLU A  51       9.269  10.607   5.305  1.00  0.75           C
ATOM    314  CD  GLU A  51       9.524  10.061   6.706  1.00  0.75           C
ATOM    315  OE1 GLU A  51      10.714   9.844   7.045  1.00  0.75
O
ATOM    316  OE2 GLU A  51       8.517   9.862   7.439  1.00  0.75           O
ATOM    317  N   GLY A  52      10.273   8.201   1.540  1.00  0.87           N
ATOM    318  CA  GLY A  52      11.160   7.402   0.692  1.00  0.87           C
ATOM    319  C   GLY A  52      10.670   7.229  -0.729  1.00  0.87           C
ATOM    320  O   GLY A  52      11.456   7.115  -1.667  1.00  0.87           O
ATOM    321  N   GLY A  53       9.334   7.190  -0.921  1.00  0.84           N
ATOM    322  CA  GLY A  53       8.691   7.201  -2.236  1.00  0.84           C
ATOM    323  C   GLY A  53       7.866   5.986  -2.579  1.00  0.84           C
ATOM    324  O   GLY A  53       7.922   4.945  -1.928  1.00  0.84           O
ATOM    325  N   LYS A  54       7.079   6.086  -3.683  1.00  0.69           N
ATOM    326  CA  LYS A  54       6.192   5.037  -4.187  1.00  0.69           C
ATOM    327  C   LYS A  54       6.879   3.707  -4.357  1.00  0.69           C
ATOM    328  O   LYS A  54       6.434   2.690  -3.846  1.00  0.69           O
ATOM    329  CB  LYS A  54       5.494   5.493  -5.488  1.00  0.69           C
ATOM    330  CG  LYS A  54       4.505   6.624  -5.168  1.00  0.69           C
ATOM    331  CD  LYS A  54       3.761   7.159  -6.403  1.00  0.69           C
ATOM    332  CE  LYS A  54       2.825   8.335  -6.103  1.00  0.69           C
ATOM    333  NZ  LYS A  54       2.072   8.722  -7.318  1.00  0.69           N
ATOM    334  N   LYS A  55       8.052   3.708  -4.994  1.00  0.64           N
ATOM    335  CA  LYS A  55       8.842   2.524  -5.188  1.00  0.64           C
ATOM    336  C   LYS A  55       9.469   1.896  -3.927  1.00  0.64           C
ATOM    337  O   LYS A  55       9.719   0.695  -3.881  1.00  0.64           O
ATOM    338  CB  LYS A  55       9.889   2.900  -6.236  1.00  0.64           C
ATOM    339  CG  LYS A  55      10.609   1.686  -6.811  1.00  0.64           C
ATOM    340  CD  LYS A  55      11.589   2.083  -7.915  1.00  0.64           C
ATOM    341  CE  LYS A  55      12.708   2.986  -7.397  1.00  0.64           C
ATOM    342  NZ  LYS A  55      13.658   3.280  -8.485  1.00  0.64           N
ATOM    343  N   ALA A  56       9.735   2.683  -2.860  1.00  0.69           N
ATOM    344  CA  ALA A  56      10.171   2.160  -1.577  1.00  0.69           C
ATOM    345  C   ALA A  56       9.072   1.367  -0.864  1.00  0.69           C
ATOM    346  O   ALA A  56       9.297   0.283  -0.335  1.00  0.69           O
ATOM    347  CB  ALA A  56      10.647   3.332  -0.697  1.00  0.69           C
ATOM    348  N   GLY A  57       7.828   1.894  -0.873  1.00  0.73           N
ATOM    349  CA  GLY A  57       6.690   1.213  -0.262  1.00  0.73           C
ATOM    350  C   GLY A  57       6.098   0.061  -1.070  1.00  0.73           C
ATOM    351  O   GLY A  57       5.291  -0.688  -0.547  1.00  0.73           O
ATOM    352  N   ILE A  58       6.474  -0.073  -2.376  1.00  0.60           N
ATOM    353  CA  ILE A  58       6.275  -1.259  -3.244  1.00  0.60           C
ATOM    354  C   ILE A  58       7.048  -2.472  -2.765  1.00  0.60           C
ATOM    355  O   ILE A  58       6.581  -3.605  -2.809  1.00  0.60           O
ATOM    356  CB  ILE A  58       6.688  -1.036  -4.725  1.00  0.60           C
ATOM    357  CG1 ILE A  58       5.666  -0.091  -5.355  1.00  0.60           C
ATOM    358  CG2 ILE A  58       6.668  -2.340  -5.557  1.00  0.60           C
ATOM    359  CD1 ILE A  58       5.847   0.438  -6.782  1.00  0.60           C
ATOM    360  N   ALA A  59       8.310  -2.225  -2.375  1.00  0.62           N
ATOM    361  CA  ALA A  59       9.219  -3.234  -1.890  1.00  0.62           C
ATOM    362  C   ALA A  59       8.973  -3.659  -0.431  1.00  0.62           C
ATOM    363  O   ALA A  59       9.284  -4.783  -0.050  1.00  0.62           O
ATOM    364  CB  ALA A  59      10.656  -2.705  -2.079  1.00  0.62           C
ATOM    365  N   PHE A  60       8.430  -2.738   0.393  1.00  0.53           N
ATOM    366  CA  PHE A  60       8.005  -2.952   1.771  1.00  0.53           C
ATOM    367  C   PHE A  60       6.703  -3.830   1.953  1.00  0.53           C
ATOM    368  O   PHE A  60       5.922  -4.011   0.980  1.00  0.53           O
ATOM    369  CB  PHE A  60       7.914  -1.519   2.392  1.00  0.53           C
ATOM    370  CG  PHE A  60       7.623  -1.510   3.865  1.00  0.53           C
ATOM    371  CD1 PHE A  60       8.612  -1.813   4.817  1.00  0.53           C
ATOM    372  CD2 PHE A  60       6.315  -1.253   4.298  1.00  0.53           C
ATOM    373  CE1 PHE A  60       8.272  -1.935   6.173  1.00  0.53           C
ATOM    374  CE2 PHE A  60       5.973  -1.377   5.648  1.00  0.53           C
ATOM    375  CZ  PHE A  60       6.950  -1.729   6.586  1.00  0.53           C
ATOM    376  OXT PHE A  60       6.499  -4.371   3.082  1.00  0.53           O
TER     377      PHE A  60
END
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B)

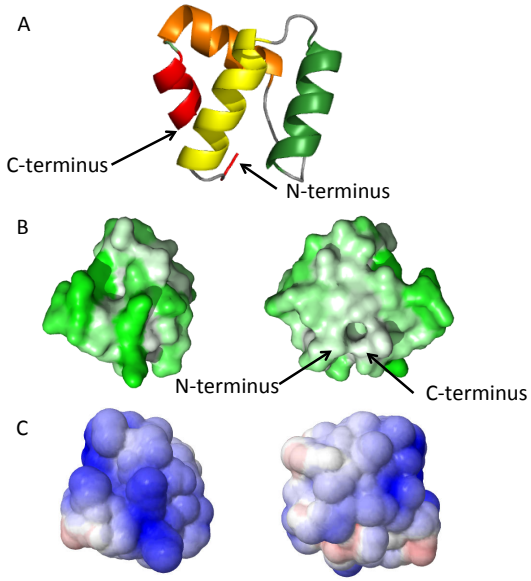

Figure S2- Structural models of aureocyclicin. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of aureocyclicin. Orientation peptide backbone in the space filling diagrams, B and C, correlate to one another.

3) Amylocyclicin

A) PDB file for model of amylocyclicin. Structure modeled after NKR-5-3B using SWISS-MODEL[84]

TITLE SWISS-MODEL SERVER (https://swissmodel.expasy.org)
TITLE 2 Untitled Project
EXPDTA THEORETICAL MODEL (SWISS-MODEL SERVER)
AUTHOR SWISS-MODEL SERVER (SEE REFERENCE IN JRNL Records)
REVDAT 1 31-OCT-16 1MOD 1 16:08
JRNL AUTH M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO CASSARINO,M.BERTONI,L.BORDOLI,
JRNL AUTH 3 T.SCHWEDE
JRNL TITL SWISS-MODEL: MODELLING PROTEIN TERTIARY AND QUATERNARY
JRNL TITL 2 STRUCTURE USING EVOLUTIONARY INFORMATION
JRNL REF NUCLEIC.ACIDS.RES 2014
JRNL REFN ISSN 0305-1048
JRNL PMID 24782522
JRNL DOI 10.1093/nar/gku340
REMARK 3
REMARK 3 MODEL INFORMATION
REMARK 3 ENGIN PROMOD3
REMARK 3 VERSN 1.0.1
REMARK 3 OSTAT MONOMER
REMARK 3 OSRSN USER
REMARK 3 GMQE 0.83
REMARK 3 QMN4 -0.46
REMARK 3 MODT FALSE
REMARK 3
REMARK 3 TEMPLATE 1
REMARK 3 PDBID 2mp8
REMARK 3 CHAIN A
REMARK 3 MMCIF A
REMARK 3 PDBV 2016-10-14
REMARK 3 SMTLE 2mp8.1.A
REMARK 3 SMTLV 2016-10-19
REMARK 3 MTHD SOLUTION NMR 0.00 A
REMARK 3 FOUND HHblits
REMARK 3 GMQE 0.83
REMARK 3 SIM 0.47
REMARK 3 SID 60.94
REMARK 3 OSTAT monomer

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ATOM      1  N   LEU A   1       5.371  -3.112   0.968  1.00  0.75           N
ATOM      2  CA  LEU A   1       4.212  -3.996   0.837  1.00  0.75           C
ATOM      3  C   LEU A   1       4.587  -5.410   0.480  1.00  0.75           C
ATOM      4  O   LEU A   1       4.199  -6.345   1.174  1.00  0.75           O
ATOM      5  CB  LEU A   1       3.359  -3.235  -0.189  1.00  0.75           C
ATOM      6  CG  LEU A   1       2.915  -1.821   0.249  1.00  0.75           C
ATOM      7  CD1 LEU A   1       2.267  -1.163  -0.971  1.00  0.75           C
ATOM      8  CD2 LEU A   1       1.987  -1.831   1.477  1.00  0.75           C
ATOM      9  N   ALA A   2       5.401  -5.638  -0.558  1.00  0.74           N
ATOM     10  CA  ALA A   2       5.742  -6.974  -0.966  1.00  0.74           C
ATOM     11  C   ALA A   2       6.433  -7.882   0.062  1.00  0.74           C
ATOM     12  O   ALA A   2       6.006  -9.032   0.246  1.00  0.74           O
ATOM     13  CB  ALA A   2       6.619  -6.845  -2.215  1.00  0.74           C
ATOM     14  N   SER A   3       7.459  -7.379   0.768  1.00  0.72           N
ATOM     15  CA  SER A   3       8.200  -8.002   1.862  1.00  0.72           C
ATOM     16  C   SER A   3       7.372  -8.176   3.127  1.00  0.72           C
ATOM     17  O   SER A   3       7.418  -9.235   3.742  1.00  0.72           O
ATOM     18  CB  SER A   3       9.465  -7.206   2.311  1.00  0.72           C
ATOM     19  OG  SER A   3      10.534  -7.167   1.355  1.00  0.72           O
ATOM     20  N   THR A   4       6.606  -7.148   3.586  1.00  0.71           N
ATOM     21  CA  THR A   4       5.831  -7.267   4.836  1.00  0.71           C
ATOM     22  C   THR A   4       4.529  -8.020   4.714  1.00  0.71           C
ATOM     23  O   THR A   4       4.101  -8.708   5.639  1.00  0.71           O
ATOM     24  CB  THR A   4       5.500  -5.973   5.573  1.00  0.71           C
ATOM     25  OG1 THR A   4       4.725  -5.054   4.797  1.00  0.71           O
ATOM     26  CG2 THR A   4       6.809  -5.290   5.972  1.00  0.71           C
ATOM     27  N   LEU A   5       3.852  -7.887   3.564  1.00  0.71           N
ATOM     28  CA  LEU A   5       2.565  -8.502   3.331  1.00  0.71           C
ATOM     29  C   LEU A   5       2.705  -9.846   2.651  1.00  0.71           C
ATOM     30  O   LEU A   5       1.805 -10.680   2.710  1.00  0.71           O
ATOM     31  CB  LEU A   5       1.709  -7.611   2.400  1.00  0.71           C
ATOM     32  CG  LEU A   5       1.529  -6.160   2.872  1.00  0.71           C
ATOM     33  CD1 LEU A   5       0.927  -5.332   1.734  1.00  0.71           C
ATOM     34  CD2 LEU A   5       0.683  -6.068   4.144  1.00  0.71           C
ATOM     35  N   GLY A   6       3.851 -10.088   1.981  1.00  0.78           N
ATOM     36  CA  GLY A   6       4.099 -11.320   1.242  1.00  0.78           C
ATOM     37  C   GLY A   6       3.324 -11.389  -0.045  1.00  0.78           C
ATOM     38  O   GLY A   6       2.790 -12.428  -0.423  1.00  0.78           O
ATOM     39  N   ILE A   7       3.240 -10.246  -0.746  1.00  0.73           N
ATOM     40  CA  ILE A   7       2.450 -10.081  -1.948  1.00  0.73           C
ATOM     41  C   ILE A   7       3.368  -9.880  -3.128  1.00  0.73           C
ATOM     42  O   ILE A   7       4.570  -9.660  -3.004  1.00  0.73           O
ATOM     43  CB  ILE A   7       1.435  -8.933  -1.894  1.00  0.73           C
ATOM     44  CG1 ILE A   7       2.102  -7.556  -1.666  1.00  0.73           C
ATOM     45  CG2 ILE A   7       0.378  -9.290  -0.828  1.00  0.73           C
ATOM     46  CD1 ILE A   7       1.132  -6.374  -1.742  1.00  0.73           C
ATOM     47  N   SER A   8       2.810  -9.966  -4.346  1.00  0.81           N
ATOM     48  CA  SER A   8       3.535  -9.702  -5.573  1.00  0.81           C
ATOM     49  C   SER A   8       3.849  -8.228  -5.758  1.00  0.81           C
ATOM     50  O   SER A   8       3.209  -7.347  -5.187  1.00  0.81           O
ATOM     51  CB  SER A   8       2.770 -10.218  -6.823  1.00  0.81           C
ATOM     52  OG  SER A   8       1.511  -9.559  -7.009  1.00  0.81           O
ATOM     53  N   THR A   9       4.848  -7.905  -6.599  1.00  0.76           N
ATOM     54  CA  THR A   9       5.168  -6.533  -6.984  1.00  0.76           C
ATOM     55  C   THR A   9       4.030  -5.873  -7.746  1.00  0.76           C
ATOM     56  O   THR A   9       3.795  -4.670  -7.637  1.00  0.76           O
ATOM     57  CB  THR A   9       6.430  -6.440  -7.828  1.00  0.76           C
ATOM     58  OG1 THR A   9       6.357  -7.276  -8.977  1.00  0.76           O
ATOM     59  CG2 THR A   9       7.628  -6.929  -7.007  1.00  0.76           C
ATOM     60  N   ALA A  10       3.273  -6.678  -8.525  1.00  0.82           N
ATOM     61  CA  ALA A  10       2.067  -6.271  -9.208  1.00  0.82           C
ATOM     62  C   ALA A  10       0.986  -5.768  -8.261  1.00  0.82           C
ATOM     63  O   ALA A  10       0.487  -4.653  -8.411  1.00  0.82           O
ATOM     64  CB  ALA A  10       1.494  -7.470  -9.995  1.00  0.82           C
ATOM     65  N   ALA A  11       0.659  -6.567  -7.221  1.00  0.84           N
ATOM     66  CA  ALA A  11      -0.270  -6.225  -6.168  1.00  0.84           C
ATOM     67  C   ALA A  11       0.226  -5.083  -5.310  1.00  0.84           C
ATOM     68  O   ALA A  11      -0.547  -4.207  -4.925  1.00  0.84           O
ATOM     69  CB  ALA A  11      -0.534  -7.444  -5.269  1.00  0.84           C
ATOM     70  N   ALA A  12       1.539  -5.046  -5.005  1.00  0.83           N
ATOM     71  CA  ALA A  12       2.150  -3.948  -4.294  1.00  0.83           C
ATOM     72  C   ALA A  12       2.018  -2.626  -5.031  1.00  0.83           C
ATOM     73  O   ALA A  12       1.532  -1.651  -4.471  1.00  0.83           O
ATOM     74  CB  ALA A  12       3.638  -4.246  -4.029  1.00  0.83           C
ATOM     75  N   LYS A  13       2.348  -2.574  -6.333  1.00  0.78           N
ATOM     76  CA  LYS A  13       2.183  -1.397  -7.169  1.00  0.78           C
ATOM     77  C   LYS A  13       0.743  -0.947  -7.312  1.00  0.78           C
ATOM     78  O   LYS A  13       0.435   0.238  -7.416  1.00  0.78           O
ATOM     79  CB  LYS A  13       2.733  -1.657  -8.581  1.00  0.78           C
ATOM     80  CG  LYS A  13       2.854  -0.387  -9.438  1.00  0.78           C
ATOM     81  CD  LYS A  13       3.412  -0.675 -10.839  1.00  0.78           C
ATOM     82  CE  LYS A  13       2.499  -1.495 -11.753  1.00  0.78           C
ATOM     83  NZ  LYS A  13       1.281  -0.718 -12.058  1.00  0.78           N
ATOM     84  N   LYS A  14      -0.191  -1.910  -7.347  1.00  0.80           N
ATOM     85  CA  LYS A  14      -1.596  -1.608  -7.229  1.00  0.80           C
ATOM     86  C   LYS A  14      -1.995  -1.024  -5.890  1.00  0.80           C
ATOM     87  O   LYS A  14      -2.712  -0.035  -5.853  1.00  0.80           O
ATOM     88  CB  LYS A  14      -2.452  -2.840  -7.544  1.00  0.80           C
ATOM     89  CG  LYS A  14      -2.402  -3.216  -9.030  1.00  0.80           C
ATOM     90  CD  LYS A  14      -3.562  -4.125  -9.454  1.00  0.80           C
ATOM     91  CE  LYS A  14      -4.941  -3.456  -9.418  1.00  0.80           C
ATOM     92  NZ  LYS A  14      -4.985  -2.274 -10.304  1.00  0.80           N
ATOM     93  N   ALA A  15      -1.501  -1.565  -4.762  1.00  0.85           N
ATOM     94  CA  ALA A  15      -1.711  -0.982  -3.454  1.00  0.85           C
ATOM     95  C   ALA A  15      -1.161   0.439  -3.360  1.00  0.85           C
ATOM     96  O   ALA A  15      -1.798   1.310  -2.775  1.00  0.85           O
ATOM     97  CB  ALA A  15      -1.052  -1.848  -2.373  1.00  0.85           C
ATOM     98  N   ILE A  16       0.009   0.697  -3.993  1.00  0.78           N
ATOM     99  CA  ILE A  16       0.617   2.018  -4.133  1.00  0.78           C
ATOM    100  C   ILE A  16      -0.289   3.040  -4.788  1.00  0.78           C
ATOM    101  O   ILE A  16      -0.435   4.141  -4.267  1.00  0.78           O
ATOM    102  CB  ILE A  16       1.937   2.005  -4.903  1.00  0.78           C
ATOM    103  CG1 ILE A  16       3.040   1.193  -4.195  1.00  0.78           C
ATOM    104  CG2 ILE A  16       2.471   3.426  -5.185  1.00  0.78           C
ATOM    105  CD1 ILE A  16       3.381   1.661  -2.785  1.00  0.78           C
ATOM    106  N   ASP A  17      -0.954   2.705  -5.911  1.00  0.80           N
ATOM    107  CA  ASP A  17      -1.905   3.587  -6.559  1.00  0.80           C
ATOM    108  C   ASP A  17      -3.056   3.931  -5.614  1.00  0.80           C
ATOM    109  O   ASP A  17      -3.422   5.088  -5.425  1.00  0.80           O
ATOM    110  CB  ASP A  17      -2.384   2.874  -7.847  1.00  0.80           C
ATOM    111  CG  ASP A  17      -3.412   3.677  -8.627  1.00  0.80           C
ATOM    112  OD1 ASP A  17      -3.004   4.662  -9.288  1.00  0.80           O
ATOM    113  OD2 ASP A  17      -4.595   3.250  -8.612  1.00  0.80           O
ATOM    114  N   ILE A  18      -3.593   2.920  -4.913  1.00  0.76           N
ATOM    115  CA  ILE A  18      -4.713   3.111  -4.014  1.00  0.76           C
ATOM    116  C   ILE A  18      -4.382   3.955  -2.791  1.00  0.76           C
ATOM    117  O   ILE A  18      -5.128   4.874  -2.450  1.00  0.76           O
ATOM    118  CB  ILE A  18      -5.293   1.789  -3.556  1.00  0.76           C
ATOM    119  CG1 ILE A  18      -5.596   0.855  -4.746  1.00  0.76           C
ATOM    120  CG2 ILE A  18      -6.586   2.055  -2.759  1.00  0.76           C
ATOM    121  CD1 ILE A  18      -5.826  -0.591  -4.308  1.00  0.76           C
ATOM    122  N   ILE A  19      -3.248   3.708  -2.106  1.00  0.76           N
ATOM    123  CA  ILE A  19      -2.803   4.494  -0.953  1.00  0.76           C
ATOM    124  C   ILE A  19      -2.416   5.916  -1.317  1.00  0.76           C
ATOM    125  O   ILE A  19      -2.462   6.800  -0.458  1.00  0.76           O
ATOM    126  CB  ILE A  19      -1.625   3.890  -0.172  1.00  0.76           C
ATOM    127  CG1 ILE A  19      -0.357   3.752  -1.036  1.00  0.76           C
ATOM    128  CG2 ILE A  19      -2.026   2.528   0.412  1.00  0.76           C
ATOM    129  CD1 ILE A  19       0.854   3.169  -0.311  1.00  0.76           C
ATOM    130  N   ASP A  20      -1.988   6.134  -2.579  1.00  0.77           N
ATOM    131  CA  ASP A  20      -1.671   7.428  -3.139  1.00  0.77           C
ATOM    132  C   ASP A  20      -2.917   8.235  -3.477  1.00  0.77           C
ATOM    133  O   ASP A  20      -3.041   9.408  -3.120  1.00  0.77           O
ATOM    134  CB  ASP A  20      -0.819   7.207  -4.415  1.00  0.77           C
ATOM    135  CG  ASP A  20      -0.208   8.490  -4.929  1.00  0.77           C
ATOM    136  OD1 ASP A  20       0.542   9.137  -4.156  1.00  0.77           O
ATOM    137  OD2 ASP A  20      -0.314   8.768  -6.155  1.00  0.77           O
ATOM    138  N   ALA A  21      -3.879   7.605  -4.180  1.00  0.75           N
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ATOM    139  CA  ALA A  21      -5.051   8.269  -4.693  1.00  0.75           C
ATOM    140  C   ALA A  21      -6.083   8.592  -3.640  1.00  0.75           C
ATOM    141  O   ALA A  21      -6.717   9.647  -3.623  1.00  0.75           O
ATOM    142  CB  ALA A  21      -5.705   7.364  -5.752  1.00  0.75           C
ATOM    143  N   ALA A  22      -6.301   7.625  -2.744  1.00  0.77           N
ATOM    144  CA  ALA A  22      -7.265   7.722  -1.699  1.00  0.77           C
ATOM    145  C   ALA A  22      -6.736   8.481  -0.498  1.00  0.77           C
ATOM    146  O   ALA A  22      -5.552   8.459  -0.168  1.00  0.77           O
ATOM    147  CB  ALA A  22      -7.679   6.297  -1.330  1.00  0.77           C
ATOM    148  N   SER A  23      -7.646   9.169   0.217  1.00  0.68           N
ATOM    149  CA  SER A  23      -7.284  10.123   1.253  1.00  0.68           C
ATOM    150  C   SER A  23      -7.472   9.526   2.628  1.00  0.68           C
ATOM    151  O   SER A  23      -6.520   9.203   3.343  1.00  0.68           O
ATOM    152  CB  SER A  23      -8.142  11.407   1.142  1.00  0.68           C
ATOM    153  OG  SER A  23      -7.820  12.074  -0.075  1.00  0.68           O
ATOM    154  N   THR A  24      -8.745   9.369   3.031  1.00  0.71           N
ATOM    155  CA  THR A  24      -9.197   8.800   4.292  1.00  0.71           C
ATOM    156  C   THR A  24      -8.743   7.376   4.471  1.00  0.71           C
ATOM    157  O   THR A  24      -8.958   6.547   3.589  1.00  0.71           O
ATOM    158  CB  THR A  24     -10.714   8.815   4.384  1.00  0.71           C
ATOM    159  OG1 THR A  24     -11.170  10.156   4.309  1.00  0.71
O
ATOM    160  CG2 THR A  24     -11.261   8.208   5.684  1.00  0.71
C
ATOM    161  N   ILE A  25      -8.147   7.026   5.634  1.00  0.67           N
ATOM    162  CA  ILE A  25      -7.600   5.698   5.890  1.00  0.67           C
ATOM    163  C   ILE A  25      -8.612   4.585   5.661  1.00  0.67           C
ATOM    164  O   ILE A  25      -8.351   3.647   4.917  1.00  0.67           O
ATOM    165  CB  ILE A  25      -7.039   5.627   7.308  1.00  0.67           C
ATOM    166  CG1 ILE A  25      -5.755   6.478   7.430  1.00  0.67           C
ATOM    167  CG2 ILE A  25      -6.777   4.172   7.756  1.00  0.67           C
ATOM    168  CD1 ILE A  25      -5.305   6.663   8.884  1.00  0.67           C
ATOM    169  N   ALA A  26      -9.829   4.716   6.222  1.00  0.76           N
ATOM    170  CA  ALA A  26     -10.908   3.762   6.075  1.00  0.76           C
ATOM    171  C   ALA A  26     -11.319   3.524   4.631  1.00  0.76           C
ATOM    172  O   ALA A  26     -11.567   2.399   4.210  1.00  0.76           O
ATOM    173  CB  ALA A  26     -12.116   4.238   6.901  1.00  0.76           C
ATOM    174  N   SER A  27     -11.342   4.605   3.826  1.00  0.76           N
ATOM    175  CA  SER A  27     -11.611   4.548   2.401  1.00  0.76           C
ATOM    176  C   SER A  27     -10.554   3.744   1.669  1.00  0.76           C
ATOM    177  O   SER A  27     -10.863   2.896   0.841  1.00  0.76           O
ATOM    178  CB  SER A  27     -11.710   5.959   1.773  1.00  0.76           C
ATOM    179  OG  SER A  27     -12.727   6.732   2.423  1.00  0.76           O
ATOM    180  N   ILE A  28      -9.267   3.968   2.013  1.00  0.71           N
ATOM    181  CA  ILE A  28      -8.122   3.252   1.457  1.00  0.71           C
ATOM    182  C   ILE A  28      -8.142   1.772   1.748  1.00  0.71           C
ATOM    183  O   ILE A  28      -7.953   0.950   0.847  1.00  0.71           O
ATOM    184  CB  ILE A  28      -6.790   3.772   1.990  1.00  0.71           C
ATOM    185  CG1 ILE A  28      -6.633   5.263   1.699  1.00  0.71           C
ATOM    186  CG2 ILE A  28      -5.661   3.069   1.241  1.00  0.71           C
ATOM    187  CD1 ILE A  28      -5.447   6.043   2.270  1.00  0.71           C
ATOM    188  N   ILE A  29      -8.403   1.399   3.014  1.00  0.70           N
ATOM    189  CA  ILE A  29      -8.423   0.022   3.492  1.00  0.70           C
ATOM    190  C   ILE A  29      -9.438  -0.784   2.722  1.00  0.70           C
ATOM    191  O   ILE A  29      -9.157  -1.878   2.230  1.00  0.70           O
ATOM    192  CB  ILE A  29      -8.811  -0.052   4.967  1.00  0.70           C
ATOM    193  CG1 ILE A  29      -7.784   0.644   5.875  1.00  0.70           C
ATOM    194  CG2 ILE A  29      -8.974  -1.520   5.426  1.00  0.70           C
ATOM    195  CD1 ILE A  29      -8.326   0.892   7.284  1.00  0.70           C
ATOM    196  N   SER A  30     -10.645  -0.205   2.555  1.00  0.77           N
ATOM    197  CA  SER A  30     -11.705  -0.831   1.794  1.00  0.77           C
ATOM    198  C   SER A  30     -11.302  -1.068   0.357  1.00  0.77           C
ATOM    199  O   SER A  30     -11.434  -2.174  -0.159  1.00  0.77           O
ATOM    200  CB  SER A  30     -13.020  -0.015   1.837  1.00  0.77           C
ATOM    201  OG  SER A  30     -13.552   0.008   3.164  1.00  0.77           O
ATOM    202  N   LEU A  31     -10.727  -0.061  -0.321  1.00  0.74           N
ATOM    203  CA  LEU A  31     -10.292  -0.203  -1.695  1.00  0.74           C
ATOM    204  C   LEU A  31      -9.155  -1.178  -1.898  1.00  0.74           C
ATOM    205  O   LEU A  31      -9.181  -1.991  -2.819  1.00  0.74           O
ATOM    206  CB  LEU A  31      -9.880   1.150  -2.290  1.00  0.74           C
ATOM    207  CG  LEU A  31     -10.993   2.205  -2.349  1.00  0.74           C
ATOM    208  CD1 LEU A  31     -10.411   3.532  -2.857  1.00  0.74
C
ATOM    209  CD2 LEU A  31     -12.206   1.755  -3.176  1.00  0.74
C
ATOM    210  N   ILE A  32      -8.131  -1.147  -1.029  1.00  0.73           N
ATOM    211  CA  ILE A  32      -7.032  -2.090  -1.094  1.00  0.73           C
ATOM    212  C   ILE A  32      -7.465  -3.516  -0.876  1.00  0.73           C
ATOM    213  O   ILE A  32      -7.085  -4.407  -1.630  1.00  0.73           O
ATOM    214  CB  ILE A  32      -5.950  -1.742  -0.111  1.00  0.73           C
ATOM    215  CG1 ILE A  32      -5.300  -0.429  -0.534  1.00  0.73           C
ATOM    216  CG2 ILE A  32      -4.875  -2.832  -0.092  1.00  0.73           C
ATOM    217  CD1 ILE A  32      -4.321   0.075   0.508  1.00  0.73           C
ATOM    218  N   GLY A  33      -8.314  -3.753   0.141  1.00  0.76           N
ATOM    219  CA  GLY A  33      -8.805  -5.087   0.445  1.00  0.76           C
ATOM    220  C   GLY A  33      -9.653  -5.700  -0.641  1.00  0.76           C
ATOM    221  O   GLY A  33      -9.634  -6.914  -0.844  1.00  0.76           O
ATOM    222  N   ILE A  34     -10.386  -4.849  -1.392  1.00  0.68           N
ATOM    223  CA  ILE A  34     -11.117  -5.195  -2.608  1.00  0.68           C
ATOM    224  C   ILE A  34     -10.182  -5.638  -3.721  1.00  0.68           C
ATOM    225  O   ILE A  34     -10.451  -6.608  -4.429  1.00  0.68           O
ATOM    226  CB  ILE A  34     -12.022  -4.043  -3.068  1.00  0.68           C
ATOM    227  CG1 ILE A  34     -13.192  -3.848  -2.077  1.00  0.68           C
ATOM    228  CG2 ILE A  34     -12.578  -4.262  -4.495  1.00  0.68           C
ATOM    229  CD1 ILE A  34     -13.941  -2.524  -2.278  1.00  0.68           C
ATOM    230  N   VAL A  35      -9.050  -4.931  -3.903  1.00  0.76           N
ATOM    231  CA  VAL A  35      -8.087  -5.215  -4.951  1.00  0.76           C
ATOM    232  C   VAL A  35      -7.189  -6.404  -4.670  1.00  0.76           C
ATOM    233  O   VAL A  35      -6.974  -7.248  -5.538  1.00  0.76           O
ATOM    234  CB  VAL A  35      -7.229  -3.991  -5.231  1.00  0.76           C
ATOM    235  CG1 VAL A  35      -6.064  -4.305  -6.192  1.00  0.76
C
ATOM    236  CG2 VAL A  35      -8.141  -2.903  -5.834  1.00  0.76
C
ATOM    237  N   THR A  36      -6.610  -6.504  -3.458  1.00  0.76           N
ATOM    238  CA  THR A  36      -5.709  -7.604  -3.137  1.00  0.76           C
ATOM    239  C   THR A  36      -6.447  -8.871  -2.764  1.00  0.76           C
ATOM    240  O   THR A  36      -5.891  -9.966  -2.839  1.00  0.76           O
ATOM    241  CB  THR A  36      -4.714  -7.301  -2.017  1.00  0.76           C
ATOM    242  OG1 THR A  36      -5.352  -6.916  -0.805  1.00  0.76
O
ATOM    243  CG2 THR A  36      -3.802  -6.140  -2.435  1.00  0.76
C
ATOM    244  N   GLY A  37      -7.733  -8.753  -2.366  1.00  0.75           N
ATOM    245  CA  GLY A  37      -8.574  -9.882  -1.994  1.00  0.75           C
ATOM    246  C   GLY A  37      -8.211 -10.452  -0.653  1.00  0.75           C
ATOM    247  O   GLY A  37      -8.321 -11.655  -0.409  1.00  0.75           O
ATOM    248  N   ALA A  38      -7.755  -9.585   0.261  1.00  0.68           N
ATOM    249  CA  ALA A  38      -7.313  -9.989   1.563  1.00  0.68           C
ATOM    250  C   ALA A  38      -7.343  -8.789   2.490  1.00  0.68           C
ATOM    251  O   ALA A  38      -7.177  -7.645   2.078  1.00  0.68           O
ATOM    252  CB  ALA A  38      -5.884 -10.576   1.487  1.00  0.68           C
ATOM    253  N   GLY A  39      -7.510  -9.026   3.809  1.00  0.64           N
ATOM    254  CA  GLY A  39      -7.517  -7.978   4.833  1.00  0.64           C
ATOM    255  C   GLY A  39      -6.144  -7.710   5.389  1.00  0.64           C
ATOM    256  O   GLY A  39      -5.995  -7.268   6.524  1.00  0.64           O
ATOM    257  N   ALA A  40      -5.101  -8.022   4.594  1.00  0.67           N
ATOM    258  CA  ALA A  40      -3.700  -7.870   4.928  1.00  0.67           C
ATOM    259  C   ALA A  40      -3.309  -6.418   5.111  1.00  0.67           C
ATOM    260  O   ALA A  40      -2.608  -6.039   6.048  1.00  0.67           O
ATOM    261  CB  ALA A  40      -2.835  -8.493   3.813  1.00  0.67           C
ATOM    262  N   ILE A  41      -3.806  -5.549   4.217  1.00  0.69           N
ATOM    263  CA  ILE A  41      -3.562  -4.135   4.307  1.00  0.69           C
ATOM    264  C   ILE A  41      -4.631  -3.534   5.189  1.00  0.69           C
ATOM    265  O   ILE A  41      -5.737  -3.186   4.776  1.00  0.69           O
ATOM    266  CB  ILE A  41      -3.499  -3.419   2.974  1.00  0.69           C
ATOM    267  CG1 ILE A  41      -2.384  -3.966   2.048  1.00  0.69           C
ATOM    268  CG2 ILE A  41      -3.261  -1.915   3.246  1.00  0.69           C
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ATOM    269  CD1 ILE A  41      -2.711  -5.240   1.253  1.00  0.69           C
ATOM    270  N   SER A  42      -4.284  -3.420   6.470  1.00  0.72           N
ATOM    271  CA  SER A  42      -5.088  -2.831   7.507  1.00  0.72           C
ATOM    272  C   SER A  42      -4.767  -1.358   7.631  1.00  0.72           C
ATOM    273  O   SER A  42      -3.936  -0.821   6.902  1.00  0.72           O
ATOM    274  CB  SER A  42      -4.838  -3.556   8.858  1.00  0.72           C
ATOM    275  OG  SER A  42      -3.547  -3.271   9.416  1.00  0.72           O
ATOM    276  N   TYR A  43      -5.387  -0.656   8.602  1.00  0.66           N
ATOM    277  CA  TYR A  43      -5.124   0.746   8.887  1.00  0.66           C
ATOM    278  C   TYR A  43      -3.650   1.052   9.141  1.00  0.66           C
ATOM    279  O   TYR A  43      -3.125   2.068   8.693  1.00  0.66           O
ATOM    280  CB  TYR A  43      -6.003   1.243  10.084  1.00  0.66           C
ATOM    281  CG  TYR A  43      -5.550   0.729  11.430  1.00  0.66           C
ATOM    282  CD1 TYR A  43      -4.620   1.471  12.176  1.00  0.66
C
ATOM    283  CD2 TYR A  43      -5.967  -0.514  11.931  1.00  0.66
C
ATOM    284  CE1 TYR A  43      -4.090   0.964  13.367  1.00  0.66           C
ATOM    285  CE2 TYR A  43      -5.453  -1.004  13.141  1.00  0.66
C
ATOM    286  CZ  TYR A  43      -4.510  -0.267  13.858  1.00  0.66           C
ATOM    287  OH  TYR A  43      -3.960  -0.760  15.059  1.00  0.66
O
ATOM    288  N   ALA A  44      -2.966   0.131   9.857  1.00  0.77           N
ATOM    289  CA  ALA A  44      -1.567   0.185  10.202  1.00  0.77           C
ATOM    290  C   ALA A  44      -0.704   0.131   8.960  1.00  0.77           C
ATOM    291  O   ALA A  44       0.225   0.910   8.785  1.00  0.77           O
ATOM    292  CB  ALA A  44      -1.232  -0.989  11.153  1.00  0.77           C
ATOM    293  N   ILE A  45      -1.036  -0.775   8.024  1.00  0.73           N
ATOM    294  CA  ILE A  45      -0.350  -0.875   6.752  1.00  0.73           C
ATOM    295  C   ILE A  45      -0.603   0.333   5.872  1.00  0.73           C
ATOM    296  O   ILE A  45       0.333   0.863   5.280  1.00  0.73           O
ATOM    297  CB  ILE A  45      -0.705  -2.147   6.009  1.00  0.73           C
ATOM    298  CG1 ILE A  45      -0.464  -3.417   6.859  1.00  0.73           C
ATOM    299  CG2 ILE A  45       0.059  -2.221   4.666  1.00  0.73           C
ATOM    300  CD1 ILE A  45       0.985  -3.621   7.310  1.00  0.73           C
ATOM    301  N   VAL A  46      -1.856   0.829   5.782  1.00  0.80           N
ATOM    302  CA  VAL A  46      -2.189   2.035   5.027  1.00  0.80           C
ATOM    303  C   VAL A  46      -1.482   3.268   5.533  1.00  0.80           C
ATOM    304  O   VAL A  46      -0.890   4.022   4.755  1.00  0.80           O
ATOM    305  CB  VAL A  46      -3.677   2.357   5.098  1.00  0.80           C
ATOM    306  CG1 VAL A  46      -4.024   3.701   4.422  1.00  0.80           C
ATOM    307  CG2 VAL A  46      -4.472   1.253   4.399  1.00  0.80           C
ATOM    308  N   ALA A  47      -1.521   3.501   6.861  1.00  0.83           N
ATOM    309  CA  ALA A  47      -0.886   4.632   7.485  1.00  0.83           C
ATOM    310  C   ALA A  47       0.616   4.584   7.287  1.00  0.83           C
ATOM    311  O   ALA A  47       1.219   5.532   6.810  1.00  0.83           O
ATOM    312  CB  ALA A  47      -1.229   4.683   8.989  1.00  0.83           C
ATOM    313  N   THR A  48       1.239   3.419   7.568  1.00  0.83           N
ATOM    314  CA  THR A  48       2.664   3.230   7.342  1.00  0.83           C
ATOM    315  C   THR A  48       3.035   3.368   5.898  1.00  0.83           C
ATOM    316  O   THR A  48       3.935   4.132   5.568  1.00  0.83           O
ATOM    317  CB  THR A  48       3.177   1.900   7.858  1.00  0.83           C
ATOM    318  OG1 THR A  48       2.913   1.792   9.248  1.00  0.83           O
ATOM    319  CG2 THR A  48       4.701   1.757   7.724  1.00  0.83           C
ATOM    320  N   ALA A  49       2.320   2.732   4.958  1.00  0.86           N
ATOM    321  CA  ALA A  49       2.645   2.811   3.559  1.00  0.86           C
ATOM    322  C   ALA A  49       2.563   4.220   2.991  1.00  0.86           C
ATOM    323  O   ALA A  49       3.486   4.669   2.318  1.00  0.86           O
ATOM    324  CB  ALA A  49       1.741   1.845   2.784  1.00  0.86           C
ATOM    325  N   LYS A  50       1.504   4.996   3.311  1.00  0.79           N
ATOM    326  CA  LYS A  50       1.417   6.374   2.867  1.00  0.79           C
ATOM    327  C   LYS A  50       2.469   7.287   3.492  1.00  0.79           C
ATOM    328  O   LYS A  50       2.895   8.283   2.908  1.00  0.79           O
ATOM    329  CB  LYS A  50       0.023   7.009   3.031  1.00  0.79           C
ATOM    330  CG  LYS A  50      -0.390   7.329   4.472  1.00  0.79           C
ATOM    331  CD  LYS A  50      -1.555   8.320   4.528  1.00  0.79           C
ATOM    332  CE  LYS A  50      -2.837   7.782   3.895  1.00  0.79           C
ATOM    333  NZ  LYS A  50      -3.829   8.867   3.783  1.00  0.79           N
ATOM    334  N   THR A  51       2.920   6.984   4.731  1.00  0.84           N
ATOM    335  CA  THR A  51       4.027   7.713   5.344  1.00  0.84           C
ATOM    336  C   THR A  51       5.341   7.396   4.684  1.00  0.84           C
ATOM    337  O   THR A  51       6.162   8.299   4.522  1.00  0.84           O
ATOM    338  CB  THR A  51       4.207   7.641   6.859  1.00  0.84           C
ATOM    339  OG1 THR A  51       4.596   6.371   7.369  1.00  0.84           O
ATOM    340  CG2 THR A  51       2.934   8.101   7.563  1.00  0.84           C
ATOM    341  N   MET A  52       5.573   6.126   4.297  1.00  0.80           N
ATOM    342  CA  MET A  52       6.719   5.654   3.539  1.00  0.80           C
ATOM    343  C   MET A  52       6.806   6.244   2.146  1.00  0.80           C
ATOM    344  O   MET A  52       7.881   6.657   1.715  1.00  0.80           O
ATOM    345  CB  MET A  52       6.779   4.112   3.415  1.00  0.80           C
ATOM    346  CG  MET A  52       6.886   3.294   4.723  1.00  0.80           C
ATOM    347  SD  MET A  52       8.332   3.563   5.779  1.00  0.80           S
ATOM    348  CE  MET A  52       7.701   4.902   6.842  1.00  0.80           C
ATOM    349  N   ILE A  53       5.679   6.353   1.411  1.00  0.77           N
ATOM    350  CA  ILE A  53       5.686   6.982   0.097  1.00  0.77           C
ATOM    351  C   ILE A  53       5.927   8.476   0.148  1.00  0.77           C
ATOM    352  O   ILE A  53       6.391   9.076  -0.816  1.00  0.77           O
ATOM    353  CB  ILE A  53       4.459   6.705  -0.771  1.00  0.77           C
ATOM    354  CG1 ILE A  53       3.198   7.417  -0.251  1.00  0.77           C
ATOM    355  CG2 ILE A  53       4.275   5.185  -0.858  1.00  0.77           C
ATOM    356  CD1 ILE A  53       1.925   7.196  -1.071  1.00  0.77           C
ATOM    357  N   LYS A  54       5.618   9.112   1.292  1.00  0.77           N
ATOM    358  CA  LYS A  54       5.920  10.504   1.520  1.00  0.77           C
ATOM    359  C   LYS A  54       7.398  10.813   1.712  1.00  0.77           C
ATOM    360  O   LYS A  54       7.902  11.798   1.174  1.00  0.77           O
ATOM    361  CB  LYS A  54       5.126  10.999   2.753  1.00  0.77           C
ATOM    362  CG  LYS A  54       5.310  12.486   3.097  1.00  0.77           C
ATOM    363  CD  LYS A  54       4.865  13.440   1.979  1.00  0.77           C
ATOM    364  CE  LYS A  54       3.373  13.413   1.657  1.00  0.77           C
ATOM    365  NZ  LYS A  54       2.620  13.945   2.810  1.00  0.77           N
ATOM    366  N   LYS A  55       8.116  10.001   2.515  1.00  0.78           N
ATOM    367  CA  LYS A  55       9.533  10.205   2.767  1.00  0.78           C
ATOM    368  C   LYS A  55      10.445   9.536   1.759  1.00  0.78           C
ATOM    369  O   LYS A  55      11.368  10.156   1.238  1.00  0.78           O
ATOM    370  CB  LYS A  55       9.956   9.781   4.203  1.00  0.78           C
ATOM    371  CG  LYS A  55       9.365   8.460   4.709  1.00  0.78           C
ATOM    372  CD  LYS A  55       9.700   8.134   6.173  1.00  0.78           C
ATOM    373  CE  LYS A  55       9.117   9.092   7.210  1.00  0.78           C
ATOM    374  NZ  LYS A  55       7.640   9.059   7.156  1.00  0.78           N
ATOM    375  N   TYR A  56      10.223   8.245   1.469  1.00  0.78           N
ATOM    376  CA  TYR A  56      11.145   7.463   0.677  1.00  0.78           C
ATOM    377  C   TYR A  56      10.659   7.308  -0.749  1.00  0.78           C
ATOM    378  O   TYR A  56      11.431   7.299  -1.707  1.00  0.78           O
ATOM    379  CB  TYR A  56      11.264   6.050   1.289  1.00  0.78           C
ATOM    380  CG  TYR A  56      11.638   6.043   2.744  1.00  0.78           C
ATOM    381  CD1 TYR A  56      12.679   6.832   3.247  1.00  0.78
C
ATOM    382  CD2 TYR A  56      10.952   5.209   3.635  1.00  0.78
C
ATOM    383  CE1 TYR A  56      12.992   6.822   4.612  1.00  0.78           C
ATOM    384  CE2 TYR A  56      11.327   5.124   4.977  1.00  0.78           C
ATOM    385  CZ  TYR A  56      12.316   5.963   5.477  1.00  0.78           C
ATOM    386  OH  TYR A  56      12.560   5.963   6.858  1.00  0.78           O
ATOM    387  N   GLY A  57       9.329   7.203  -0.917  1.00  0.89           N
ATOM    388  CA  GLY A  57       8.694   7.192  -2.221  1.00  0.89           C
ATOM    389  C   GLY A  57       7.858   5.975  -2.481  1.00  0.89           C
ATOM    390  O   GLY A  57       7.917   4.953  -1.800  1.00  0.89           O
ATOM    391  N   LYS A  58       7.031   6.060  -3.535  1.00  0.76           N
ATOM    392  CA  LYS A  58       6.108   5.020  -3.949  1.00  0.76           C
ATOM    393  C   LYS A  58       6.746   3.673  -4.216  1.00  0.76           C
ATOM    394  O   LYS A  58       6.278   2.622  -3.790  1.00  0.76           O
ATOM    395  CB  LYS A  58       5.419   5.499  -5.227  1.00  0.76           C
ATOM    396  CG  LYS A  58       4.438   6.633  -4.962  1.00  0.76           C
ATOM    397  CD  LYS A  58       3.808   7.083  -6.281  1.00  0.76           C
ATOM    398  CE  LYS A  58       2.815   8.200  -6.010  1.00  0.76           C
ATOM    399  NZ  LYS A  58       2.040   8.615  -7.193  1.00  0.76           N
ATOM    400  N   LYS A  59       7.891   3.698  -4.905  1.00  0.74           N
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ATOM    401  CA  LYS A  59       8.678   2.526  -5.201  1.00  0.74           C
ATOM    402  C   LYS A  59       9.297   1.852  -3.979  1.00  0.74           C
ATOM    403  O   LYS A  59       9.439   0.631  -3.933  1.00  0.74           O
ATOM    404  CB  LYS A  59       9.763   2.913  -6.218  1.00  0.74           C
ATOM    405  CG  LYS A  59      10.534   1.711  -6.775  1.00  0.74           C
ATOM    406  CD  LYS A  59      11.528   2.100  -7.877  1.00  0.74           C
ATOM    407  CE  LYS A  59      12.664   2.993  -7.373  1.00  0.74           C
ATOM    408  NZ  LYS A  59      13.621   3.281  -8.464  1.00  0.74           N
ATOM    409  N   TYR A  60       9.672   2.640  -2.943  1.00  0.73           N
ATOM    410  CA  TYR A  60      10.147   2.103  -1.681  1.00  0.73           C
ATOM    411  C   TYR A  60       9.045   1.316  -1.008  1.00  0.73           C
ATOM    412  O   TYR A  60       9.221   0.177  -0.583  1.00  0.73           O
ATOM    413  CB  TYR A  60      10.582   3.257  -0.735  1.00  0.73           C
ATOM    414  CG  TYR A  60      10.969   2.759   0.636  1.00  0.73           C
ATOM    415  CD1 TYR A  60       9.993   2.560   1.627  1.00  0.73           C
ATOM    416  CD2 TYR A  60      12.291   2.418   0.922  1.00  0.73
C
ATOM    417  CE1 TYR A  60      10.326   1.985   2.857  1.00  0.73           C
ATOM    418  CE2 TYR A  60      12.634   1.883   2.171  1.00  0.73           C
ATOM    419  CZ  TYR A  60      11.650   1.665   3.139  1.00  0.73           C
ATOM    420  OH  TYR A  60      11.978   1.136   4.399  1.00  0.73           O
ATOM    421  N   ALA A  61       7.845   1.928  -0.919  1.00  0.83           N
ATOM    422  CA  ALA A  61       6.727   1.299  -0.271  1.00  0.83           C
ATOM    423  C   ALA A  61       6.279   0.047  -1.009  1.00  0.83           C
ATOM    424  O   ALA A  61       5.865  -0.907  -0.399  1.00  0.83           O
ATOM    425  CB  ALA A  61       5.554   2.258  -0.038  1.00  0.83           C
ATOM    426  N   ALA A  62       6.420   0.008  -2.359  1.00  0.81           N
ATOM    427  CA  ALA A  62       6.133  -1.176  -3.138  1.00  0.81           C
ATOM    428  C   ALA A  62       6.975  -2.370  -2.670  1.00  0.81           C
ATOM    429  O   ALA A  62       6.441  -3.444  -2.388  1.00  0.81           O
ATOM    430  CB  ALA A  62       6.379  -0.867  -4.633  1.00  0.81           C
ATOM    431  N   ALA A  63       8.294  -2.146  -2.479  1.00  0.74           N
ATOM    432  CA  ALA A  63       9.259  -3.120  -1.984  1.00  0.74           C
ATOM    433  C   ALA A  63       9.173  -3.550  -0.517  1.00  0.74           C
ATOM    434  O   ALA A  63       9.517  -4.701  -0.227  1.00  0.74           O
ATOM    435  CB  ALA A  63      10.698  -2.625  -2.198  1.00  0.74           C
ATOM    436  N   TRP A  64       8.777  -2.622   0.402  1.00  0.68           N
ATOM    437  CA  TRP A  64       8.705  -2.737   1.859  1.00  0.68           C
ATOM    438  C   TRP A  64       7.778  -3.883   2.319  1.00  0.68           C
ATOM    439  O   TRP A  64       7.558  -4.851   1.569  1.00  0.68           O
ATOM    440  CB  TRP A  64       8.153  -1.391   2.462  1.00  0.68           C
ATOM    441  CG  TRP A  64       7.682  -1.295   3.939  1.00  0.68           C
ATOM    442  CD1 TRP A  64       8.478  -1.452   5.032  1.00  0.68           C
ATOM    443  CD2 TRP A  64       6.315  -1.328   4.454  1.00  0.68           C
ATOM    444  NE1 TRP A  64       7.729  -1.553   6.184  1.00  0.68           N
ATOM    445  CE2 TRP A  64       6.402  -1.510   5.845  1.00  0.68           C
ATOM    446  CE3 TRP A  64       5.065  -1.252   3.833  1.00  0.68           C
ATOM    447  CZ2 TRP A  64       5.263  -1.632   6.634  1.00  0.68           C
ATOM    448  CZ3 TRP A  64       3.917  -1.357   4.635  1.00  0.68           C
ATOM    449  CH2 TRP A  64       4.013  -1.554   6.012  1.00  0.68           C
ATOM    450  OXT TRP A  64       7.105  -3.771   3.364  1.00  0.68           O
TER     451      TRP A  64
END
```

B)

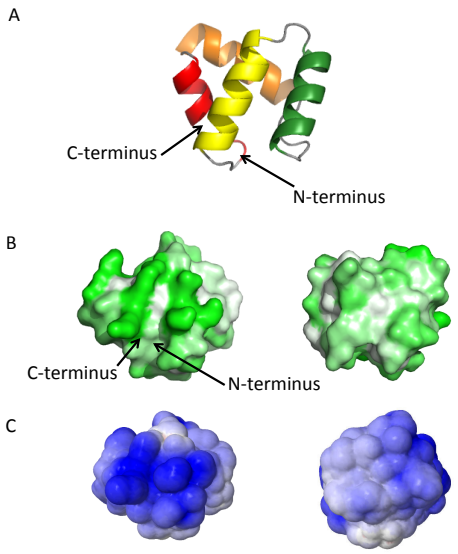

Figure S3- Structural models of amylocyclicin. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of amylocyclicin. Orientation peptide backbone in surface filling diagrams, B and C, correlate to one another.

4. Leucocyclicin

A) PDB file for model of leucocyclicin. Structure modeled after NKR-5-3B using SWISS-MODEL[84]

```
TITLE     SWISS-MODEL SERVER (https://swissmodel.expasy.org)                EXPDTA    THEORETICAL MODEL (SWISS-MODEL SERVER)
TITLE     2 Untitled Project
```

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AUTHOR    SWISS-MODEL SERVER (SEE REFERENCE IN JRNL
Records)
REVDAT   1   11-AUG-16 1MOD    1       23:52
JRNL        AUTH
M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL        AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO
CASSARINO,M.BERTONI,L.BORDOLI,
JRNL        AUTH 3 T.SCHWEDE
JRNL        TITL   SWISS-MODEL: MODELLING PROTEIN TERTIARY
AND QUATERNARY
JRNL        TITL 2 STRUCTURE USING EVOLUTIONARY
INFORMATION
JRNL        REF    NUCLEIC.ACIDS.RES                2014
JRNL        REFN                ISSN 0305-1048
JRNL        PMID   24782522
JRNL        DOI    10.1093/nar/gku340
REMARK   3
REMARK   3 MODEL INFORMATION
REMARK   3  ENGIN   PROMOD3
REMARK   3  VERSN   1.0.0
REMARK   3  OSTAT   MONOMER
REMARK   3  OSRSN   PREDICTION
REMARK   3  GMQE    0.66
REMARK   3  QMN4    -1.92
REMARK   3
REMARK   3 TEMPLATE 1
REMARK   3  PDBID   2mp8
REMARK   3  CHAIN   A
REMARK   3  MMCIF   A
REMARK   3  PDBV    2016-07-29
REMARK   3  SMTLE   2mp8.1.A
REMARK   3  SMTLV   2016-08-03
REMARK   3  MTHD    SOLUTION NMR 0.00 A
REMARK   3  FOUND   HHblits
REMARK   3  GMQE    0.66
REMARK   3  SIM     0.36
REMARK   3  SID     31.67
REMARK   3  OSTAT   monomer
ATOM      1  N   VAL A   4       5.370  -5.541  -0.615  1.00  0.72           N
ATOM      2  CA  VAL A   4       5.883  -6.910  -0.994  1.00  0.72           C
ATOM      3  C   VAL A   4       6.449  -7.673   0.163  1.00  0.72           C
ATOM      4  O   VAL A   4       5.908  -8.714   0.519  1.00  0.72           O
ATOM      5  CB  VAL A   4       6.841  -6.860  -2.184  1.00  0.72           C
ATOM      6  CG1 VAL A   4       7.445  -8.224  -2.592  1.00  0.72           C
ATOM      7  CG2 VAL A   4       6.030  -6.366  -3.384  1.00  0.72           C
ATOM      8  N   ASN A   5       7.514  -7.163   0.800  1.00  0.70           N
ATOM      9  CA  ASN A   5       8.191  -7.839   1.891  1.00  0.70           C
ATOM     10  C   ASN A   5       7.354  -8.123   3.135  1.00  0.70           C
ATOM     11  O   ASN A   5       7.357  -9.241   3.637  1.00  0.70           O
ATOM     12  CB  ASN A   5       9.401  -6.995   2.343  1.00  0.70           C
ATOM     13  CG  ASN A   5      10.461  -6.974   1.250  1.00  0.70           C
ATOM     14  OD1 ASN A   5      10.573  -7.870   0.413  1.00  0.70           O
ATOM     15  ND2 ASN A   5      11.301  -5.913   1.258  1.00  0.70           N
ATOM     16  N   GLN A   6       6.611  -7.141   3.671  1.00  0.75           N
ATOM     17  CA  GLN A   6       5.860  -7.321   4.900  1.00  0.75           C
ATOM     18  C   GLN A   6       4.523  -8.021   4.732  1.00  0.75           C
ATOM     19  O   GLN A   6       4.044  -8.711   5.627  1.00  0.75           O
ATOM     20  CB  GLN A   6       5.616  -5.947   5.560  1.00  0.75           C
ATOM     21  CG  GLN A   6       6.912  -5.224   5.994  1.00  0.75           C
ATOM     22  CD  GLN A   6       7.666  -6.028   7.049  1.00  0.75           C
ATOM     23  OE1 GLN A   6       7.120  -6.429   8.076  1.00  0.75           O
ATOM     24  NE2 GLN A   6       8.976  -6.271   6.809  1.00  0.75           N
ATOM     25  N   LEU A   7       3.878  -7.859   3.564  1.00  0.72           N
ATOM     26  CA  LEU A   7       2.585  -8.463   3.302  1.00  0.72           C
ATOM     27  C   LEU A   7       2.708  -9.826   2.631  1.00  0.72           C
ATOM     28  O   LEU A   7       1.779 -10.627   2.660  1.00  0.72           O
ATOM     29  CB  LEU A   7       1.756  -7.553   2.356  1.00  0.72           C
ATOM     30  CG  LEU A   7       1.557  -6.099   2.832  1.00  0.72           C
ATOM     31  CD1 LEU A   7       0.942  -5.250   1.707  1.00  0.72           C
ATOM     32  CD2 LEU A   7       0.706  -6.024   4.108  1.00  0.72           C
ATOM     33  N   GLY A   8       3.863 -10.123   1.994  1.00  0.84           N
ATOM     34  CA  GLY A   8       4.078 -11.358   1.238  1.00  0.84           C
ATOM     35  C   GLY A   8       3.291 -11.435  -0.053  1.00  0.84           C
ATOM     36  O   GLY A   8       2.777 -12.482  -0.433  1.00  0.84           O
ATOM     37  N   ILE A   9       3.178 -10.295  -0.762  1.00  0.74           N
ATOM     38  CA  ILE A   9       2.358 -10.123  -1.953  1.00  0.74           C
ATOM     39  C   ILE A   9       3.261  -9.955  -3.155  1.00  0.74           C
ATOM     40  O   ILE A   9       4.470  -9.792  -3.030  1.00  0.74           O
ATOM     41  CB  ILE A   9       1.389  -8.937  -1.886  1.00  0.74           C
ATOM     42  CG1 ILE A   9       2.096  -7.573  -1.668  1.00  0.74           C
ATOM     43  CG2 ILE A   9       0.341  -9.282  -0.809  1.00  0.74           C
ATOM     44  CD1 ILE A   9       1.145  -6.372  -1.740  1.00  0.74           C
ATOM     45  N   SER A  10       2.716  -9.983  -4.385  1.00  0.84           N
ATOM     46  CA  SER A  10       3.498  -9.716  -5.582  1.00  0.84           C
ATOM     47  C   SER A  10       3.818  -8.237  -5.768  1.00  0.84           C
ATOM     48  O   SER A  10       3.170  -7.356  -5.205  1.00  0.84           O
ATOM     49  CB  SER A  10       2.815 -10.254  -6.872  1.00  0.84           C
ATOM     50  OG  SER A  10       1.608  -9.550  -7.183  1.00  0.84           O
ATOM     51  N   LYS A  11       4.836  -7.912  -6.598  1.00  0.75           N
ATOM     52  CA  LYS A  11       5.141  -6.542  -6.998  1.00  0.75           C
ATOM     53  C   LYS A  11       4.009  -5.882  -7.773  1.00  0.75           C
ATOM     54  O   LYS A  11       3.780  -4.682  -7.657  1.00  0.75           O
ATOM     55  CB  LYS A  11       6.451  -6.462  -7.812  1.00  0.75           C
ATOM     56  CG  LYS A  11       7.688  -6.849  -6.989  1.00  0.75           C
ATOM     57  CD  LYS A  11       8.973  -6.781  -7.829  1.00  0.75           C
ATOM     58  CE  LYS A  11      10.235  -7.150  -7.042  1.00  0.75           C
ATOM     59  NZ  LYS A  11      11.427  -7.101  -7.920  1.00  0.75           N
ATOM     60  N   SER A  12       3.258  -6.688  -8.555  1.00  0.80           N
ATOM     61  CA  SER A  12       2.033  -6.277  -9.237  1.00  0.80           C
ATOM     62  C   SER A  12       0.972  -5.789  -8.262  1.00  0.80           C
ATOM     63  O   SER A  12       0.479  -4.668  -8.358  1.00  0.80           O
ATOM     64  CB  SER A  12       1.435  -7.471 -10.037  1.00  0.80           C
ATOM     65  OG  SER A  12       0.272  -7.104 -10.780  1.00  0.80           O
ATOM     66  N   LEU A  13       0.665  -6.598  -7.223  1.00  0.74           N
ATOM     67  CA  LEU A  13      -0.262  -6.215  -6.176  1.00  0.74           C
ATOM     68  C   LEU A  13       0.219  -5.013  -5.384  1.00  0.74           C
ATOM     69  O   LEU A  13      -0.549  -4.105  -5.102  1.00  0.74           O
ATOM     70  CB  LEU A  13      -0.545  -7.394  -5.216  1.00  0.74           C
ATOM     71  CG  LEU A  13      -1.354  -8.558  -5.825  1.00  0.74           C
ATOM     72  CD1 LEU A  13      -1.357  -9.751  -4.856  1.00  0.74           C
ATOM     73  CD2 LEU A  13      -2.793  -8.151  -6.180  1.00  0.74           C
ATOM     74  N   ALA A  14       1.510  -4.950  -5.033  1.00  0.80           N
ATOM     75  CA  ALA A  14       2.100  -3.826  -4.340  1.00  0.80           C
ATOM     76  C   ALA A  14       2.080  -2.489  -5.070  1.00  0.80           C
ATOM     77  O   ALA A  14       1.812  -1.452  -4.472  1.00  0.80           O
ATOM     78  CB  ALA A  14       3.539  -4.194  -4.023  1.00  0.80           C
ATOM     79  N   ASN A  15       2.340  -2.481  -6.388  1.00  0.75           N
ATOM     80  CA  ASN A  15       2.139  -1.334  -7.252  1.00  0.75           C
ATOM     81  C   ASN A  15       0.660  -0.912  -7.330  1.00  0.75           C
ATOM     82  O   ASN A  15       0.310   0.266  -7.333  1.00  0.75           O
ATOM     83  CB  ASN A  15       2.721  -1.677  -8.640  1.00  0.75           C
ATOM     84  CG  ASN A  15       2.786  -0.425  -9.501  1.00  0.75           C
ATOM     85  OD1 ASN A  15       3.420   0.567  -9.143  1.00  0.75           O
ATOM     86  ND2 ASN A  15       2.100  -0.448 -10.664  1.00  0.75
N
ATOM     87  N   THR A  16      -0.264  -1.885  -7.368  1.00  0.75           N
ATOM     88  CA  THR A  16      -1.702  -1.639  -7.239  1.00  0.75           C
ATOM     89  C   THR A  16      -2.102  -1.044  -5.891  1.00  0.75           C
ATOM     90  O   THR A  16      -2.887  -0.096  -5.825  1.00  0.75           O
ATOM     91  CB  THR A  16      -2.510  -2.892  -7.528  1.00  0.75           C
ATOM     92  OG1 THR A  16      -2.318  -3.274  -8.883  1.00  0.75           O
ATOM     93  CG2 THR A  16      -4.016  -2.666  -7.365  1.00  0.75           C
ATOM     94  N   ILE A  17      -1.528  -1.543  -4.769  1.00  0.69           N
ATOM     95  CA  ILE A  17      -1.676  -0.970  -3.424  1.00  0.69           C
ATOM     96  C   ILE A  17      -1.184   0.439  -3.400  1.00  0.69           C
ATOM     97  O   ILE A  17      -1.841   1.343  -2.892  1.00  0.69           O
ATOM     98  CB  ILE A  17      -0.878  -1.709  -2.344  1.00  0.69           C
ATOM     99  CG1 ILE A  17      -1.422  -3.121  -2.103  1.00  0.69           C
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ATOM    100  CG2 ILE A  17      -0.855  -0.967  -0.982  1.00  0.69           C
ATOM    101  CD1 ILE A  17      -2.854  -3.128  -1.569  1.00  0.69           C
ATOM    102  N   LEU A  18      -0.019   0.654  -4.015  1.00  0.71           N
ATOM    103  CA  LEU A  18       0.584   1.939  -4.108  1.00  0.71           C
ATOM    104  C   LEU A  18      -0.272   2.977  -4.796  1.00  0.71           C
ATOM    105  O   LEU A  18      -0.383   4.117  -4.348  1.00  0.71           O
ATOM    106  CB  LEU A  18       1.861   1.830  -4.907  1.00  0.71           C
ATOM    107  CG  LEU A  18       2.514   3.186  -5.125  1.00  0.71           C
ATOM    108  CD1 LEU A  18       2.984   3.670  -3.759  1.00  0.71           C
ATOM    109  CD2 LEU A  18       3.571   2.978  -6.199  1.00  0.71           C
ATOM    110  N   GLY A  19      -0.909   2.601  -5.918  1.00  0.75           N
ATOM    111  CA  GLY A  19      -1.873   3.471  -6.562  1.00  0.75           C
ATOM    112  C   GLY A  19      -3.050   3.777  -5.676  1.00  0.75           C
ATOM    113  O   GLY A  19      -3.453   4.928  -5.567  1.00  0.75           O
ATOM    114  N   ALA A  20      -3.604   2.780  -4.962  1.00  0.66           N
ATOM    115  CA  ALA A  20      -4.708   3.019  -4.056  1.00  0.66           C
ATOM    116  C   ALA A  20      -4.378   3.942  -2.877  1.00  0.66           C
ATOM    117  O   ALA A  20      -5.067   4.941  -2.691  1.00  0.66           O
ATOM    118  CB  ALA A  20      -5.274   1.675  -3.559  1.00  0.66           C
ATOM    119  N   ILE A  21      -3.272   3.682  -2.132  1.00  0.62           N
ATOM    120  CA  ILE A  21      -2.791   4.477  -0.993  1.00  0.62           C
ATOM    121  C   ILE A  21      -2.391   5.888  -1.377  1.00  0.62           C
ATOM    122  O   ILE A  21      -2.423   6.804  -0.569  1.00  0.62           O
ATOM    123  CB  ILE A  21      -1.640   3.825  -0.210  1.00  0.62           C
ATOM    124  CG1 ILE A  21      -0.348   3.702  -1.047  1.00  0.62           C
ATOM    125  CG2 ILE A  21      -2.144   2.470   0.326  1.00  0.62           C
ATOM    126  CD1 ILE A  21       0.855   3.117  -0.309  1.00  0.62           C
ATOM    127  N   ALA A  22      -1.962   6.084  -2.635  1.00  0.68           N
ATOM    128  CA  ALA A  22      -1.636   7.378  -3.178  1.00  0.68           C
ATOM    129  C   ALA A  22      -2.834   8.214  -3.619  1.00  0.68           C
ATOM    130  O   ALA A  22      -2.795   9.441  -3.566  1.00  0.68           O
ATOM    131  CB  ALA A  22      -0.744   7.154  -4.410  1.00  0.68           C
ATOM    132  N   VAL A  23      -3.879   7.561  -4.169  1.00  0.56           N
ATOM    133  CA  VAL A  23      -5.071   8.221  -4.688  1.00  0.56           C
ATOM    134  C   VAL A  23      -6.101   8.539  -3.629  1.00  0.56           C
ATOM    135  O   VAL A  23      -6.694   9.618  -3.617  1.00  0.56           O
ATOM    136  CB  VAL A  23      -5.753   7.374  -5.763  1.00  0.56           C
ATOM    137  CG1 VAL A  23      -7.117   7.961  -6.193  1.00  0.56           C
ATOM    138  CG2 VAL A  23      -4.848   7.331  -7.004  1.00  0.56           C
ATOM    139  N   GLY A  24      -6.410   7.583  -2.734  1.00  0.51           N
ATOM    140  CA  GLY A  24      -7.413   7.838  -1.716  1.00  0.51           C
ATOM    141  C   GLY A  24      -6.818   8.583  -0.559  1.00  0.51           C
ATOM    142  O   GLY A  24      -5.615   8.576  -0.351  1.00  0.51           O
ATOM    143  N   ASN A  25      -7.691   9.234   0.225  1.00  0.40           N
ATOM    144  CA  ASN A  25      -7.292  10.152   1.270  1.00  0.40           C
ATOM    145  C   ASN A  25      -7.539   9.542   2.635  1.00  0.40           C
ATOM    146  O   ASN A  25      -6.645   9.275   3.426  1.00  0.40           O
ATOM    147  CB  ASN A  25      -8.158  11.435   1.165  1.00  0.40           C
ATOM    148  CG  ASN A  25      -7.773  12.248  -0.066  1.00  0.40           C
ATOM    149  OD1 ASN A  25      -6.626  12.323  -0.488  1.00  0.40
O
ATOM    150  ND2 ASN A  25      -8.774  12.944  -0.658  1.00  0.40
N
ATOM    151  N   LEU A  26      -8.824   9.343   2.988  1.00  0.34           N
ATOM    152  CA  LEU A  26      -9.196   8.756   4.255  1.00  0.34           C
ATOM    153  C   LEU A  26      -8.717   7.318   4.416  1.00  0.34           C
ATOM    154  O   LEU A  26      -8.910   6.481   3.538  1.00  0.34           O
ATOM    155  CB  LEU A  26     -10.730   8.789   4.434  1.00  0.34           C
ATOM    156  CG  LEU A  26     -11.342  10.199   4.522  1.00  0.34
C
ATOM    157  CD1 LEU A  26     -12.874  10.100   4.488  1.00  0.34
C
ATOM    158  CD2 LEU A  26     -10.879  10.946   5.781  1.00  0.34
C
ATOM    159  N   ALA A  27      -8.131   6.977   5.583  1.00  0.53           N
ATOM    160  CA  ALA A  27      -7.590   5.657   5.844  1.00  0.53           C
ATOM    161  C   ALA A  27      -8.612   4.529   5.739  1.00  0.53           C
ATOM    162  O   ALA A  27      -8.342   3.459   5.216  1.00  0.53           O
ATOM    163  CB  ALA A  27      -6.971   5.634   7.255  1.00  0.53           C
ATOM    164  N   SER A  28      -9.845   4.744   6.220  1.00  0.42           N
ATOM    165  CA  SER A  28     -10.942   3.799   6.067  1.00  0.42           C
ATOM    166  C   SER A  28     -11.363   3.552   4.620  1.00  0.42           C
ATOM    167  O   SER A  28     -11.683   2.430   4.243  1.00  0.42           O
ATOM    168  CB  SER A  28     -12.169   4.237   6.906  1.00  0.42           C
ATOM    169  OG  SER A  28     -12.584   5.559   6.557  1.00  0.42           O
ATOM    170  N   TRP A  29     -11.357   4.607   3.778  1.00  0.36           N
ATOM    171  CA  TRP A  29     -11.642   4.561   2.351  1.00  0.36           C
ATOM    172  C   TRP A  29     -10.618   3.747   1.556  1.00  0.36           C
ATOM    173  O   TRP A  29     -10.949   2.965   0.666  1.00  0.36           O
ATOM    174  CB  TRP A  29     -11.715   6.013   1.813  1.00  0.36           C
ATOM    175  CG  TRP A  29     -12.090   6.136   0.352  1.00  0.36           C
ATOM    176  CD1 TRP A  29     -11.284   6.288  -0.742  1.00  0.36
C
ATOM    177  CD2 TRP A  29     -13.428   6.008  -0.136  1.00  0.36
C
ATOM    178  NE1 TRP A  29     -12.042   6.298  -1.891  1.00  0.36
N
ATOM    179  CE2 TRP A  29     -13.363   6.118  -1.542  1.00  0.36           C
ATOM    180  CE3 TRP A  29     -14.635   5.795   0.519  1.00  0.36           C
ATOM    181  CZ2 TRP A  29     -14.512   6.027  -2.311  1.00  0.36           C
ATOM    182  CZ3 TRP A  29     -15.795   5.711  -0.258  1.00  0.36           C
ATOM    183  CH2 TRP A  29     -15.737   5.830  -1.654  1.00  0.36
C
ATOM    184  N   LEU A  30      -9.327   3.903   1.901  1.00  0.47           N
ATOM    185  CA  LEU A  30      -8.200   3.183   1.340  1.00  0.47           C
ATOM    186  C   LEU A  30      -8.189   1.664   1.577  1.00  0.47           C
ATOM    187  O   LEU A  30      -7.350   0.953   1.026  1.00  0.47           O
ATOM    188  CB  LEU A  30      -6.889   3.779   1.916  1.00  0.47           C
ATOM    189  CG  LEU A  30      -6.500   5.186   1.436  1.00  0.47           C
ATOM    190  CD1 LEU A  30      -5.231   5.713   2.134  1.00  0.47           C
ATOM    191  CD2 LEU A  30      -6.240   5.047  -0.054  1.00  0.47           C
ATOM    192  N   LEU A  31      -9.142   1.118   2.367  1.00  0.46           N
ATOM    193  CA  LEU A  31      -9.217  -0.293   2.717  1.00  0.46           C
ATOM    194  C   LEU A  31     -10.094  -1.078   1.759  1.00  0.46           C
ATOM    195  O   LEU A  31     -10.405  -2.243   2.008  1.00  0.46           O
ATOM    196  CB  LEU A  31      -9.794  -0.525   4.141  1.00  0.46           C
ATOM    197  CG  LEU A  31      -8.912  -0.006   5.288  1.00  0.46           C
ATOM    198  CD1 LEU A  31      -9.661  -0.082   6.625  1.00  0.46           C
ATOM    199  CD2 LEU A  31      -7.615  -0.810   5.400  1.00  0.46           C
ATOM    200  N   ALA A  32     -10.505  -0.497   0.607  1.00  0.47           N
ATOM    201  CA  ALA A  32     -11.161  -1.251  -0.449  1.00  0.47
C
ATOM    202  C   ALA A  32     -10.151  -2.125  -1.182  1.00  0.47           C
ATOM    203  O   ALA A  32      -9.722  -1.877  -2.310  1.00  0.47           O
ATOM    204  CB  ALA A  32     -11.953  -0.368  -1.434  1.00  0.47
C
ATOM    205  N   LEU A  33      -9.711  -3.188  -0.502  1.00  0.48           N
ATOM    206  CA  LEU A  33      -8.689  -4.066  -0.987  1.00  0.48           C
ATOM    207  C   LEU A  33      -9.102  -4.972  -2.154  1.00  0.48           C
ATOM    208  O   LEU A  33      -9.581  -6.091  -1.989  1.00  0.48           O
ATOM    209  CB  LEU A  33      -8.044  -4.847   0.181  1.00  0.48           C
ATOM    210  CG  LEU A  33      -7.443  -3.963   1.298  1.00  0.48           C
ATOM    211  CD1 LEU A  33      -6.979  -4.889   2.425  1.00  0.48           C
ATOM    212  CD2 LEU A  33      -6.313  -3.028   0.829  1.00  0.48           C
ATOM    213  N   VAL A  34      -8.768  -4.506  -3.382  1.00  0.53           N
ATOM    214  CA  VAL A  34      -8.574  -5.320  -4.595  1.00  0.53           C
ATOM    215  C   VAL A  34      -7.645  -6.514  -4.476  1.00  0.53           C
ATOM    216  O   VAL A  34      -7.989  -7.522  -5.094  1.00  0.53           O
ATOM    217  CB  VAL A  34      -8.124  -4.559  -5.855  1.00  0.53           C
ATOM    218  CG1 VAL A  34      -8.119  -5.483  -7.108  1.00  0.53
C
ATOM    219  CG2 VAL A  34      -9.082  -3.386  -6.099  1.00  0.53
C
ATOM    220  N   PRO A  35      -6.518  -6.550  -3.755  1.00  0.62           N
ATOM    221  CA  PRO A  35      -5.822  -7.795  -3.474  1.00  0.62           C
ATOM    222  C   PRO A  35      -6.704  -9.049  -3.224  1.00  0.62           C
ATOM    223  O   PRO A  35      -6.283 -10.136  -3.609  1.00  0.62           O
ATOM    224  CB  PRO A  35      -4.845  -7.374  -2.340  1.00  0.62           C
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ATOM    225  CG  PRO A  35      -4.561  -5.883  -2.502  1.00  0.62           C
ATOM    226  CD  PRO A  35      -5.876  -5.398  -3.088  1.00  0.62           C
ATOM    227  N   GLY A  36      -7.890  -8.930  -2.556  1.00  0.51           N
ATOM    228  CA  GLY A  36      -8.751 -10.010  -2.058  1.00  0.51
C
ATOM    229  C   GLY A  36      -8.529 -10.530  -0.622  1.00  0.51           C
ATOM    230  O   GLY A  36      -9.325 -11.366  -0.202  1.00  0.51           O
ATOM    231  N   PRO A  37      -7.536 -10.094   0.188  1.00  0.50           N
ATOM    232  CA  PRO A  37      -7.497 -10.278   1.635  1.00  0.50           C
ATOM    233  C   PRO A  37      -7.485  -8.960   2.428  1.00  0.50           C
ATOM    234  O   PRO A  37      -7.319  -7.873   1.875  1.00  0.50           O
ATOM    235  CB  PRO A  37      -6.109 -10.903   1.802  1.00  0.50           C
ATOM    236  CG  PRO A  37      -5.245 -10.098   0.841  1.00  0.50           C
ATOM    237  CD  PRO A  37      -6.197  -9.863  -0.300  1.00  0.50           C
ATOM    238  N   GLY A  38      -7.617  -9.068   3.775  1.00  0.54           N
ATOM    239  CA  GLY A  38      -7.541  -7.985   4.767  1.00  0.54           C
ATOM    240  C   GLY A  38      -6.151  -7.723   5.312  1.00  0.54           C
ATOM    241  O   GLY A  38      -6.002  -7.287   6.449  1.00  0.54           O
ATOM    242  N   TRP A  39      -5.094  -8.030   4.528  1.00  0.52           N
ATOM    243  CA  TRP A  39      -3.688  -7.842   4.897  1.00  0.52           C
ATOM    244  C   TRP A  39      -3.283  -6.387   5.079  1.00  0.52           C
ATOM    245  O   TRP A  39      -2.550  -6.031   6.001  1.00  0.52           O
ATOM    246  CB  TRP A  39      -2.717  -8.463   3.846  1.00  0.52           C
ATOM    247  CG  TRP A  39      -2.638  -9.979   3.841  1.00  0.52           C
ATOM    248  CD1 TRP A  39      -2.952 -10.820   2.815  1.00  0.52
C
ATOM    249  CD2 TRP A  39      -2.047 -10.812   4.848  1.00  0.52
C
ATOM    250  NE1 TRP A  39      -2.930 -12.123   3.244  1.00  0.52
N
ATOM    251  CE2 TRP A  39      -2.295 -12.151   4.455  1.00  0.52           C
ATOM    252  CE3 TRP A  39      -1.296 -10.527   5.982  1.00  0.52           C
ATOM    253  CZ2 TRP A  39      -1.823 -13.205   5.201  1.00  0.52           C
ATOM    254  CZ3 TRP A  39      -0.716 -11.604   6.664  1.00  0.52           C
ATOM    255  CH2 TRP A  39      -0.983 -12.927   6.284  1.00  0.52
C
ATOM    256  N   ALA A  40      -3.743  -5.491   4.187  1.00  0.68           N
ATOM    257  CA  ALA A  40      -3.446  -4.086   4.306  1.00  0.68           C
ATOM    258  C   ALA A  40      -4.471  -3.402   5.186  1.00  0.68           C
ATOM    259  O   ALA A  40      -5.478  -2.876   4.730  1.00  0.68           O
ATOM    260  CB  ALA A  40      -3.373  -3.411   2.928  1.00  0.68           C
ATOM    261  N   THR A  41      -4.212  -3.406   6.499  1.00  0.64           N
ATOM    262  CA  THR A  41      -5.039  -2.812   7.529  1.00  0.64           C
ATOM    263  C   THR A  41      -4.749  -1.336   7.645  1.00  0.64           C
ATOM    264  O   THR A  41      -3.927  -0.778   6.923  1.00  0.64           O
ATOM    265  CB  THR A  41      -4.832  -3.489   8.878  1.00  0.64           C
ATOM    266  OG1 THR A  41      -3.450  -3.561   9.216  1.00  0.64
O
ATOM    267  CG2 THR A  41      -5.366  -4.918   8.751  1.00  0.64           C
ATOM    268  N   LYS A  42      -5.417  -0.632   8.581  1.00  0.63           N
ATOM    269  CA  LYS A  42      -5.145   0.770   8.863  1.00  0.63           C
ATOM    270  C   LYS A  42      -3.685   1.061   9.199  1.00  0.63           C
ATOM    271  O   LYS A  42      -3.139   2.085   8.798  1.00  0.63           O
ATOM    272  CB  LYS A  42      -5.993   1.234  10.063  1.00  0.63           C
ATOM    273  CG  LYS A  42      -7.494   1.304   9.761  1.00  0.63           C
ATOM    274  CD  LYS A  42      -8.283   1.763  10.997  1.00  0.63           C
ATOM    275  CE  LYS A  42      -9.787   1.868  10.738  1.00  0.63           C
ATOM    276  NZ  LYS A  42     -10.505   2.272  11.969  1.00  0.63           N
ATOM    277  N   ALA A  43      -3.029   0.133   9.930  1.00  0.73           N
ATOM    278  CA  ALA A  43      -1.613   0.174  10.224  1.00  0.73           C
ATOM    279  C   ALA A  43      -0.752   0.107   8.966  1.00  0.73           C
ATOM    280  O   ALA A  43       0.170   0.897   8.789  1.00  0.73           O
ATOM    281  CB  ALA A  43      -1.252  -0.995  11.169  1.00  0.73           C
ATOM    282  N   ALA A  44      -1.061  -0.811   8.024  1.00  0.76           N
ATOM    283  CA  ALA A  44      -0.361  -0.901   6.760  1.00  0.76           C
ATOM    284  C   ALA A  44      -0.566   0.312   5.868  1.00  0.76           C
ATOM    285  O   ALA A  44       0.388   0.826   5.295  1.00  0.76           O
ATOM    286  CB  ALA A  44      -0.766  -2.174   6.000  1.00  0.76           C
ATOM    287  N   LEU A  45      -1.803   0.828   5.758  1.00  0.69           N
ATOM    288  CA  LEU A  45      -2.087   2.040   5.016  1.00  0.69           C
ATOM    289  C   LEU A  45      -1.399   3.289   5.523  1.00  0.69           C
ATOM    290  O   LEU A  45      -0.764   4.012   4.758  1.00  0.69           O
ATOM    291  CB  LEU A  45      -3.575   2.361   5.124  1.00  0.69           C
ATOM    292  CG  LEU A  45      -4.513   1.405   4.397  1.00  0.69           C
ATOM    293  CD1 LEU A  45      -5.893   1.955   4.704  1.00  0.69           C
ATOM    294  CD2 LEU A  45      -4.280   1.404   2.886  1.00  0.69           C
ATOM    295  N   ALA A  46      -1.487   3.545   6.845  1.00  0.76           N
ATOM    296  CA  ALA A  46      -0.866   4.687   7.477  1.00  0.76           C
ATOM    297  C   ALA A  46       0.646   4.648   7.343  1.00  0.76           C
ATOM    298  O   ALA A  46       1.292   5.631   6.986  1.00  0.76           O
ATOM    299  CB  ALA A  46      -1.233   4.710   8.974  1.00  0.76           C
ATOM    300  N   THR A  47       1.253   3.469   7.585  1.00  0.81           N
ATOM    301  CA  THR A  47       2.683   3.277   7.385  1.00  0.81           C
ATOM    302  C   THR A  47       3.089   3.429   5.934  1.00  0.81           C
ATOM    303  O   THR A  47       4.021   4.162   5.623  1.00  0.81           O
ATOM    304  CB  THR A  47       3.168   1.923   7.880  1.00  0.81           C
ATOM    305  OG1 THR A  47       2.894   1.788   9.265  1.00  0.81           O
ATOM    306  CG2 THR A  47       4.688   1.764   7.756  1.00  0.81           C
ATOM    307  N   ALA A  48       2.369   2.792   4.988  1.00  0.82           N
ATOM    308  CA  ALA A  48       2.670   2.856   3.576  1.00  0.82           C
ATOM    309  C   ALA A  48       2.568   4.257   2.989  1.00  0.82           C
ATOM    310  O   ALA A  48       3.484   4.696   2.302  1.00  0.82           O
ATOM    311  CB  ALA A  48       1.769   1.870   2.813  1.00  0.82           C
ATOM    312  N   GLU A  49       1.508   5.035   3.295  1.00  0.73           N
ATOM    313  CA  GLU A  49       1.408   6.421   2.863  1.00  0.73           C
ATOM    314  C   GLU A  49       2.523   7.324   3.431  1.00  0.73           C
ATOM    315  O   GLU A  49       3.089   8.194   2.765  1.00  0.73           O
ATOM    316  CB  GLU A  49       0.011   7.013   3.105  1.00  0.73           C
ATOM    317  CG  GLU A  49      -0.139   8.391   2.415  1.00  0.73           C
ATOM    318  CD  GLU A  49      -1.492   9.059   2.640  1.00  0.73           C
ATOM    319  OE1 GLU A  49      -2.388   8.421   3.246  1.00  0.73           O
ATOM    320  OE2 GLU A  49      -1.581  10.262   2.268  1.00  0.73
O
ATOM    321  N   THR A  50       2.920   7.100   4.695  1.00  0.80           N
ATOM    322  CA  THR A  50       4.081   7.746   5.321  1.00  0.80           C
ATOM    323  C   THR A  50       5.411   7.377   4.673  1.00  0.80           C
ATOM    324  O   THR A  50       6.264   8.234   4.435  1.00  0.80           O
ATOM    325  CB  THR A  50       4.129   7.494   6.819  1.00  0.80           C
ATOM    326  OG1 THR A  50       2.978   8.068   7.425  1.00  0.80           O
ATOM    327  CG2 THR A  50       5.315   8.186   7.504  1.00  0.80           C
ATOM    328  N   ILE A  51       5.614   6.090   4.315  1.00  0.73           N
ATOM    329  CA  ILE A  51       6.752   5.618   3.523  1.00  0.73           C
ATOM    330  C   ILE A  51       6.796   6.274   2.155  1.00  0.73           C
ATOM    331  O   ILE A  51       7.835   6.780   1.731  1.00  0.73           O
ATOM    332  CB  ILE A  51       6.761   4.097   3.366  1.00  0.73           C
ATOM    333  CG1 ILE A  51       7.002   3.415   4.728  1.00  0.73           C
ATOM    334  CG2 ILE A  51       7.856   3.635   2.373  1.00  0.73           C
ATOM    335  CD1 ILE A  51       6.733   1.909   4.684  1.00  0.73           C
ATOM    336  N   VAL A  52       5.659   6.365   1.432  1.00  0.75           N
ATOM    337  CA  VAL A  52       5.671   6.996   0.117  1.00  0.75           C
ATOM    338  C   VAL A  52       5.878   8.492   0.150  1.00  0.75           C
ATOM    339  O   VAL A  52       6.277   9.093  -0.844  1.00  0.75           O
ATOM    340  CB  VAL A  52       4.466   6.714  -0.771  1.00  0.75           C
ATOM    341  CG1 VAL A  52       4.249   5.207  -0.854  1.00  0.75           C
ATOM    342  CG2 VAL A  52       3.194   7.357  -0.221  1.00  0.75           C
ATOM    343  N   LYS A  53       5.601   9.127   1.300  1.00  0.72           N
ATOM    344  CA  LYS A  53       5.924  10.510   1.539  1.00  0.72           C
ATOM    345  C   LYS A  53       7.411  10.808   1.723  1.00  0.72           C
ATOM    346  O   LYS A  53       7.915  11.775   1.160  1.00  0.72           O
ATOM    347  CB  LYS A  53       5.134  10.997   2.777  1.00  0.72           C
ATOM    348  CG  LYS A  53       5.309  12.488   3.109  1.00  0.72           C
ATOM    349  CD  LYS A  53       4.847  13.438   1.988  1.00  0.72           C
ATOM    350  CE  LYS A  53       3.352  13.389   1.661  1.00  0.72           C
ATOM    351  NZ  LYS A  53       2.576  13.875   2.820  1.00  0.72           N
ATOM    352  N   HIS A  54       8.137  10.003   2.532  1.00  0.70           N
ATOM    353  CA  HIS A  54       9.556  10.224   2.787  1.00  0.70           C
ATOM    354  C   HIS A  54      10.472   9.542   1.775  1.00  0.70           C
ATOM    355  O   HIS A  54      11.336  10.165   1.166  1.00  0.70           O
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ATOM    356  CB  HIS A  54       9.922   9.707   4.205  1.00  0.70           C
ATOM    357  CG  HIS A  54      11.365   9.869   4.579  1.00  0.70           C
ATOM    358  ND1 HIS A  54      11.866  11.143   4.737  1.00  0.70           N
ATOM    359  CD2 HIS A  54      12.353   8.950   4.737  1.00  0.70           C
ATOM    360  CE1 HIS A  54      13.149  10.979   4.980  1.00  0.70           C
ATOM    361  NE2 HIS A  54      13.499   9.670   4.993  1.00  0.70           N
ATOM    362  N   GLU A  55      10.306   8.221   1.576  1.00  0.69           N
ATOM    363  CA  GLU A  55      11.189   7.419   0.745  1.00  0.69           C
ATOM    364  C   GLU A  55      10.711   7.350  -0.675  1.00  0.69           C
ATOM    365  O   GLU A  55      11.478   7.397  -1.636  1.00  0.69           O
ATOM    366  CB  GLU A  55      11.258   5.981   1.285  1.00  0.69           C
ATOM    367  CG  GLU A  55      11.956   5.912   2.655  1.00  0.69           C
ATOM    368  CD  GLU A  55      12.040   4.499   3.224  1.00  0.69           C
ATOM    369  OE1 GLU A  55      11.447   3.569   2.620  1.00  0.69
O
ATOM    370  OE2 GLU A  55      12.695   4.354   4.287  1.00  0.69
O
ATOM    371  N   GLY A  56       9.387   7.244  -0.839  1.00  0.78           N
ATOM    372  CA  GLY A  56       8.785   7.281  -2.145  1.00  0.78           C
ATOM    373  C   GLY A  56       7.963   6.085  -2.426  1.00  0.78           C
ATOM    374  O   GLY A  56       7.970   5.058  -1.752  1.00  0.78           O
ATOM    375  N   LYS A  57       7.193   6.218  -3.501  1.00  0.71           N
ATOM    376  CA  LYS A  57       6.244   5.237  -3.943  1.00  0.71           C
ATOM    377  C   LYS A  57       6.852   3.851  -4.196  1.00  0.71           C
ATOM    378  O   LYS A  57       6.369   2.840  -3.693  1.00  0.71           O
ATOM    379  CB  LYS A  57       5.578   5.824  -5.204  1.00  0.71           C
ATOM    380  CG  LYS A  57       4.579   6.959  -4.925  1.00  0.71           C
ATOM    381  CD  LYS A  57       3.755   7.242  -6.192  1.00  0.71           C
ATOM    382  CE  LYS A  57       2.664   8.291  -5.978  1.00  0.71           C
ATOM    383  NZ  LYS A  57       2.026   8.658  -7.261  1.00  0.71           N
ATOM    384  N   ALA A  58       7.998   3.796  -4.904  1.00  0.73           N
ATOM    385  CA  ALA A  58       8.769   2.597  -5.168  1.00  0.73           C
ATOM    386  C   ALA A  58       9.374   1.902  -3.939  1.00  0.73           C
ATOM    387  O   ALA A  58       9.546   0.684  -3.921  1.00  0.73           O
ATOM    388  CB  ALA A  58       9.845   2.930  -6.223  1.00  0.73           C
ATOM    389  N   ALA A  59       9.703   2.658  -2.872  1.00  0.75           N
ATOM    390  CA  ALA A  59      10.153   2.108  -1.609  1.00  0.75           C
ATOM    391  C   ALA A  59       9.061   1.310  -0.890  1.00  0.75           C
ATOM    392  O   ALA A  59       9.268   0.178  -0.454  1.00  0.75           O
ATOM    393  CB  ALA A  59      10.608   3.275  -0.724  1.00  0.75           C
ATOM    394  N   ALA A  60       7.832   1.877  -0.829  1.00  0.79           N
ATOM    395  CA  ALA A  60       6.671   1.247  -0.221  1.00  0.79           C
ATOM    396  C   ALA A  60       6.136   0.059  -1.003  1.00  0.79           C
ATOM    397  O   ALA A  60       5.514  -0.831  -0.435  1.00  0.79           O
ATOM    398  CB  ALA A  60       5.503   2.232  -0.055  1.00  0.79           C
ATOM    399  N   ILE A  61       6.372   0.016  -2.337  1.00  0.70           N
ATOM    400  CA  ILE A  61       6.154  -1.176  -3.156  1.00  0.70           C
ATOM    401  C   ILE A  61       6.993  -2.345  -2.659  1.00  0.70           C
ATOM    402  O   ILE A  61       6.480  -3.439  -2.432  1.00  0.70           O
ATOM    403  CB  ILE A  61       6.471  -0.929  -4.644  1.00  0.70           C
ATOM    404  CG1 ILE A  61       5.414  -0.016  -5.300  1.00  0.70           C
ATOM    405  CG2 ILE A  61       6.559  -2.246  -5.461  1.00  0.70           C
ATOM    406  CD1 ILE A  61       5.777   0.388  -6.736  1.00  0.70           C
ATOM    407  N   ALA A  62       8.309  -2.139  -2.444  1.00  0.73           N
ATOM    408  CA  ALA A  62       9.190  -3.161  -1.921  1.00  0.73           C
ATOM    409  C   ALA A  62       8.861  -3.576  -0.487  1.00  0.73           C
ATOM    410  O   ALA A  62       8.795  -4.770  -0.188  1.00  0.73           O
ATOM    411  CB  ALA A  62      10.654  -2.695  -2.067  1.00  0.73           C
ATOM    412  N   TRP A  63       8.591  -2.599   0.400  1.00  0.65           N
ATOM    413  CA  TRP A  63       8.145  -2.812   1.767  1.00  0.65           C
ATOM    414  C   TRP A  63       6.893  -3.747   1.873  1.00  0.65           C
ATOM    415  O   TRP A  63       5.913  -3.583   1.089  1.00  0.65           O
ATOM    416  CB  TRP A  63       7.961  -1.418   2.442  1.00  0.65           C
ATOM    417  CG  TRP A  63       7.620  -1.450   3.920  1.00  0.65           C
ATOM    418  CD1 TRP A  63       8.446  -1.520   5.006  1.00  0.65           C
ATOM    419  CD2 TRP A  63       6.278  -1.449   4.426  1.00  0.65           C
ATOM    420  NE1 TRP A  63       7.702  -1.589   6.166  1.00  0.65           N
ATOM    421  CE2 TRP A  63       6.368  -1.556   5.831  1.00  0.65           C
ATOM    422  CE3 TRP A  63       5.047  -1.389   3.785  1.00  0.65           C
ATOM    423  CZ2 TRP A  63       5.222  -1.628   6.611  1.00  0.65           C
ATOM    424  CZ3 TRP A  63       3.894  -1.448   4.575  1.00  0.65           C
ATOM    425  CH2 TRP A  63       3.978  -1.571   5.968  1.00  0.65           C
ATOM    426  OXT TRP A  63       6.946  -4.704   2.692  1.00  0.65           O
TER     427      TRP A  63
END
```

B)

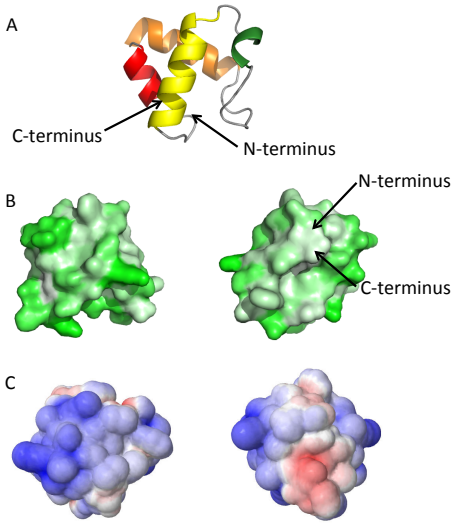

Figure S4- Structural models of leucocyclicin. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of leucocyclicin. Orientation peptide backbone in surface filling diagrams, B and C, correlate to one another.

5. Garvacin ML

A) PDB file for model of garvacin ML. Structure modeled after AS-48 using SWISS-MODEL[84]

TITLE SWISS-MODEL SERVER (https://swissmodel.expasy.org)
TITLE 2 Untitled Project
EXPDTA THEORETICAL MODEL (SWISS-MODEL SERVER)
AUTHOR SWISS-MODEL SERVER (SEE REFERENCE IN JRNL Records)
REVDAT 1 11-AUG-16 1MOD 1 22:28
JRNL AUTH
M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO
CASSARINO,M.BERTONI,L.BORDOLI,
JRNL AUTH 3 T.SCHWEDE
JRNL TITL SWISS-MODEL: MODELLING PROTEIN TERTIARY AND QUATERNARY
JRNL TITL 2 STRUCTURE USING EVOLUTIONARY INFORMATION
JRNL REF NUCLEIC.ACIDS.RES 2014
JRNL REFN ISSN 0305-1048
JRNL PMID 24782522
JRNL DOI 10.1093/nar/gku340
REMARK 3
REMARK 3 MODEL INFORMATION
REMARK 3 ENGIN PROMOD3
REMARK 3 VERSN 1.0.0
REMARK 3 OSTAT MONOMER
REMARK 3 OSRSN PREDICTION
REMARK 3 GMQE 0.65
REMARK 3 QMN4 -1.90
REMARK 3
REMARK 3 TEMPLATE 1
REMARK 3 PDBID 4rgd
REMARK 3 CHAIN A
REMARK 3 MMCIF A
REMARK 3 PDBV 2016-07-29
REMARK 3 SMTLE 4rgd.1.A
REMARK 3 SMTLV 2016-08-03
REMARK 3 MTHD X-RAY DIFFRACTION 1.20 A
REMARK 3 FOUND HHblits
REMARK 3 GMQE 0.65
REMARK 3 SIM 0.37
REMARK 3 SID 35.71
REMARK 3 OSTAT homo-dimer
REMARK 3 LIGND CIT
ATOM 1 N THR A 4 55.986 -2.970 89.102 1.00 0.34 N
ATOM 2 CA THR A 4 55.526 -2.404 87.777 1.00 0.34 C
ATOM 3 C THR A 4 56.617 -2.286 86.715 1.00 0.34 C
ATOM 4 O THR A 4 56.298 -2.050 85.596 1.00 0.34 O
ATOM 5 CB THR A 4 54.855 -1.023 87.967 1.00 0.34 C
ATOM 6 OG1 THR A 4 55.684 -0.173 88.743 1.00 0.34 O
ATOM 7 CG2 THR A 4 53.540 -1.159 88.758 1.00 0.34 C
ATOM 8 N GLY A 5 57.944 -2.498 87.008 1.00 0.40 N
ATOM 9 CA GLY A 5 58.934 -2.311 85.933 1.00 0.40 C
ATOM 10 C GLY A 5 59.203 -0.881 85.550 1.00 0.40 C
ATOM 11 O GLY A 5 59.780 -0.607 84.506 1.00 0.40 O
ATOM 12 N MET A 6 58.809 0.081 86.409 1.00 0.53 N
ATOM 13 CA MET A 6 59.205 1.459 86.267 1.00 0.53 C
ATOM 14 C MET A 6 60.640 1.570 86.645 1.00 0.53 C
ATOM 15 O MET A 6 61.020 1.242 87.759 1.00 0.53 O
ATOM 16 CB MET A 6 58.385 2.407 87.176 1.00 0.53 C

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ATOM     17  CG  MET A   6      56.907   2.378  86.776  1.00  0.53           C
ATOM     18  SD  MET A   6      56.614   2.668  85.020  1.00  0.53           S
ATOM     19  CE  MET A   6      57.503   4.240  84.995  1.00  0.53           C
ATOM     20  N   ALA A   7      61.481   2.006  85.688  1.00  0.66           N
ATOM     21  CA  ALA A   7      62.888   2.200  85.943  1.00  0.66           C
ATOM     22  C   ALA A   7      63.110   3.205  87.073  1.00  0.66           C
ATOM     23  O   ALA A   7      62.441   4.238  87.123  1.00  0.66           O
ATOM     24  CB  ALA A   7      63.618   2.670  84.660  1.00  0.66           C
ATOM     25  N   ALA A   8      64.047   2.947  88.014  1.00  0.72           N
ATOM     26  CA  ALA A   8      64.193   3.736  89.230  1.00  0.72           C
ATOM     27  C   ALA A   8      64.433   5.223  88.987  1.00  0.72           C
ATOM     28  O   ALA A   8      63.907   6.076  89.688  1.00  0.72           O
ATOM     29  CB  ALA A   8      65.318   3.164  90.121  1.00  0.72           C
ATOM     30  N   GLY A   9      65.202   5.573  87.930  1.00  0.79           N
ATOM     31  CA  GLY A   9      65.378   6.960  87.505  1.00  0.79           C
ATOM     32  C   GLY A   9      64.102   7.644  87.070  1.00  0.79           C
ATOM     33  O   GLY A   9      63.872   8.792  87.433  1.00  0.79           O
ATOM     34  N   VAL A  10      63.214   6.938  86.339  1.00  0.74           N
ATOM     35  CA  VAL A  10      61.884   7.413  85.976  1.00  0.74           C
ATOM     36  C   VAL A  10      60.982   7.511  87.196  1.00  0.74           C
ATOM     37  O   VAL A  10      60.324   8.530  87.400  1.00  0.74           O
ATOM     38  CB  VAL A  10      61.231   6.534  84.906  1.00  0.74           C
ATOM     39  CG1 VAL A  10      59.819   7.061  84.547  1.00  0.74
C
ATOM     40  CG2 VAL A  10      62.131   6.544  83.652  1.00  0.74
C
ATOM     41  N   ALA A  11      60.966   6.492  88.085  1.00  0.78           N
ATOM     42  CA  ALA A  11      60.175   6.481  89.305  1.00  0.78           C
ATOM     43  C   ALA A  11      60.522   7.630  90.264  1.00  0.78           C
ATOM     44  O   ALA A  11      59.640   8.278  90.817  1.00  0.78           O
ATOM     45  CB  ALA A  11      60.329   5.126  90.032  1.00  0.78           C
ATOM     46  N   LYS A  12      61.833   7.950  90.424  1.00  0.75           N
ATOM     47  CA  LYS A  12      62.322   9.117  91.152  1.00  0.75           C
ATOM     48  C   LYS A  12      61.795  10.433  90.584  1.00  0.75           C
ATOM     49  O   LYS A  12      61.321  11.291  91.308  1.00  0.75           O
ATOM     50  CB  LYS A  12      63.876   9.208  91.088  1.00  0.75           C
ATOM     51  CG  LYS A  12      64.606   8.168  91.954  1.00  0.75           C
ATOM     52  CD  LYS A  12      66.102   8.010  91.619  1.00  0.75           C
ATOM     53  CE  LYS A  12      66.895   9.317  91.722  1.00  0.75           C
ATOM     54  NZ  LYS A  12      68.298   9.093  91.316  1.00  0.75           N
ATOM     55  N   THR A  13      61.845  10.583  89.235  1.00  0.83           N
ATOM     56  CA  THR A  13      61.332  11.751  88.511  1.00  0.83
C
ATOM     57  C   THR A  13      59.864  11.946  88.719  1.00  0.83           C
ATOM     58  O   THR A  13      59.395  13.057  88.963  1.00  0.83           O
ATOM     59  CB  THR A  13      61.559  11.662  87.008  1.00  0.83           C
ATOM     60  OG1 THR A  13      62.951  11.721  86.766  1.00  0.83
O
ATOM     61  CG2 THR A  13      60.943  12.833  86.214  1.00  0.83
C
ATOM     62  N   ILE A  14      59.088  10.850  88.671  1.00  0.77           N
ATOM     63  CA  ILE A  14      57.683  10.908  88.994  1.00  0.77           C
ATOM     64  C   ILE A  14      57.403  11.367  90.406  1.00  0.77           C
ATOM     65  O   ILE A  14      56.600  12.266  90.622  1.00  0.77           O
ATOM     66  CB  ILE A  14      57.029   9.541  88.871  1.00  0.77           C
ATOM     67  CG1 ILE A  14      57.085   9.064  87.398  1.00  0.77           C
ATOM     68  CG2 ILE A  14      55.606   9.654  89.489  1.00  0.77           C
ATOM     69  CD1 ILE A  14      56.231   9.880  86.440  1.00  0.77           C
ATOM     70  N   VAL A  15      58.038  10.725  91.414  1.00  0.81           N
ATOM     71  CA  VAL A  15      57.756  10.990  92.819  1.00  0.81
C
ATOM     72  C   VAL A  15      58.099  12.432  93.124  1.00  0.81           C
ATOM     73  O   VAL A  15      57.383  13.116  93.869  1.00  0.81           O
ATOM     74  CB  VAL A  15      58.440   9.989  93.751  1.00  0.81           C
ATOM     75  CG1 VAL A  15      58.298  10.437  95.222  1.00  0.81
C
ATOM     76  CG2 VAL A  15      57.773   8.606  93.568  1.00  0.81
C
ATOM     77  N   ASN A  16      59.148  12.974  92.491  1.00  0.82           N
ATOM     78  CA  ASN A  16      59.478  14.383  92.532  1.00  0.82
C
ATOM     79  C   ASN A  16      58.404  15.312  91.948  1.00  0.82           C
ATOM     80  O   ASN A  16      58.130  16.371  92.474  1.00  0.82           O
ATOM     81  CB  ASN A  16      60.833  14.676  91.851  1.00  0.82           C
ATOM     82  CG  ASN A  16      61.962  14.110  92.710  1.00  0.82
C
ATOM     83  OD1 ASN A  16      61.818  13.773  93.871  1.00  0.82
O
ATOM     84  ND2 ASN A  16      63.178  14.056  92.104  1.00  0.82
N
ATOM     85  N   ALA A  17      57.746  14.921  90.829  1.00  0.84           N
ATOM     86  CA  ALA A  17      56.565  15.627  90.353  1.00  0.84
C
ATOM     87  C   ALA A  17      55.393  15.578  91.338  1.00  0.84           C
ATOM     88  O   ALA A  17      54.733  16.587  91.587  1.00  0.84           O
ATOM     89  CB  ALA A  17      56.112  15.057  88.989  1.00  0.84
C
ATOM     90  N   VAL A  18      55.135  14.415  91.964  1.00  0.80           N
ATOM     91  CA  VAL A  18      54.136  14.243  93.014  1.00  0.80
C
ATOM     92  C   VAL A  18      54.393  15.107  94.245  1.00  0.80           C
ATOM     93  O   VAL A  18      53.485  15.756  94.762  1.00  0.80           O
ATOM     94  CB  VAL A  18      54.089  12.786  93.469  1.00  0.80
C
ATOM     95  CG1 VAL A  18      53.212  12.584  94.725  1.00  0.80
C
ATOM     96  CG2 VAL A  18      53.553  11.938  92.302  1.00  0.80
C
ATOM     97  N   SER A  19      55.649  15.139  94.745  1.00  0.83           N
ATOM     98  CA  SER A  19      56.071  15.920  95.902  1.00  0.83           C
ATOM     99  C   SER A  19      56.032  17.420  95.667  1.00  0.83           C
ATOM    100  O   SER A  19      55.714  18.185  96.568  1.00  0.83           O
ATOM    101  CB  SER A  19      57.469  15.505  96.456  1.00  0.83
C
ATOM    102  OG  SER A  19      58.526  15.804  95.545  1.00  0.83
O
ATOM    103  N   ALA A  20      56.320  17.863  94.425  1.00  0.82           N
ATOM    104  CA  ALA A  20      56.237  19.249  94.020  1.00  0.82
C
ATOM    105  C   ALA A  20      54.803  19.713  93.761  1.00  0.82           C
ATOM    106  O   ALA A  20      54.554  20.908  93.595  1.00  0.82           O
ATOM    107  CB  ALA A  20      57.105  19.441  92.754  1.00  0.82
C
ATOM    108  N   GLY A  21      53.815  18.788  93.716  1.00  0.85           N
ATOM    109  CA  GLY A  21      52.417  19.111  93.440  1.00  0.85
C
ATOM    110  C   GLY A  21      52.148  19.421  91.994  1.00  0.85           C
ATOM    111  O   GLY A  21      51.234  20.160  91.669  1.00  0.85           O
ATOM    112  N   MET A  22      52.983  18.838  91.106  1.00  0.75
N
ATOM    113  CA  MET A  22      52.852  18.881  89.662  1.00  0.75
C
ATOM    114  C   MET A  22      51.628  18.141  89.155  1.00  0.75           C
ATOM    115  O   MET A  22      50.863  17.511  89.888  1.00  0.75
O
ATOM    116  CB  MET A  22      54.115  18.320  88.943  1.00  0.75
C
ATOM    117  CG  MET A  22      55.412  19.086  89.275  1.00  0.75
C
ATOM    118  SD  MET A  22      55.450  20.831  88.767  1.00  0.75
S
ATOM    119  CE  MET A  22      55.504  20.515  86.981  1.00  0.75
C
ATOM    120  N   ASP A  23      51.401  18.221  87.840  1.00  0.70           N
ATOM    121  CA  ASP A  23      50.156  17.815  87.246  1.00  0.70
C
ATOM    122  C   ASP A  23      49.999  16.300  87.134  1.00  0.70           C
ATOM    123  O   ASP A  23      50.939  15.567  86.801  1.00  0.70           O
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ATOM    124  CB  ASP A  23      50.037  18.461  85.841  1.00  0.70
C
ATOM    125  CG  ASP A  23      49.961  19.979  85.931  1.00  0.70
C
ATOM    126  OD1 ASP A  23      49.578  20.496  87.005  1.00  0.70
O
ATOM    127  OD2 ASP A  23      50.282  20.619  84.901  1.00  0.70
O
ATOM    128  N   ILE A  24      48.759  15.782  87.316  1.00  0.64           N
ATOM    129  CA  ILE A  24      48.393  14.400  87.007  1.00  0.64           C
ATOM    130  C   ILE A  24      48.657  14.059  85.547  1.00  0.64           C
ATOM    131  O   ILE A  24      49.160  12.986  85.248  1.00  0.64           O
ATOM    132  CB  ILE A  24      46.940  14.062  87.375  1.00  0.64           C
ATOM    133  CG1 ILE A  24      46.811  13.893  88.907  1.00  0.64
C
ATOM    134  CG2 ILE A  24      46.469  12.768  86.653  1.00  0.64
C
ATOM    135  CD1 ILE A  24      45.358  13.696  89.361  1.00  0.64
C
ATOM    136  N   ALA A  25      48.369  14.983  84.598  1.00  0.73           N
ATOM    137  CA  ALA A  25      48.602  14.755  83.181  1.00  0.73
C
ATOM    138  C   ALA A  25      50.076  14.490  82.860  1.00  0.73           C
ATOM    139  O   ALA A  25      50.395  13.631  82.042  1.00  0.73           O
ATOM    140  CB  ALA A  25      48.062  15.929  82.332  1.00  0.73
C
ATOM    141  N   THR A  26      51.000  15.197  83.548  1.00  0.74           N
ATOM    142  CA  THR A  26      52.447  14.989  83.477  1.00  0.74
C
ATOM    143  C   THR A  26      52.877  13.659  84.044  1.00  0.74           C
ATOM    144  O   THR A  26      53.685  12.949  83.461  1.00  0.74           O
ATOM    145  CB  THR A  26      53.243  16.065  84.195  1.00  0.74
C
ATOM    146  OG1 THR A  26      52.851  17.328  83.689  1.00  0.74
O
ATOM    147  CG2 THR A  26      54.747  15.936  83.901  1.00  0.74
C
ATOM    148  N   ALA A  27      52.313  13.253  85.207  1.00  0.76           N
ATOM    149  CA  ALA A  27      52.549  11.925  85.737  1.00  0.76
C
ATOM    150  C   ALA A  27      52.056  10.852  84.768  1.00  0.76           C
ATOM    151  O   ALA A  27      52.806   9.954  84.398  1.00  0.76           O
ATOM    152  CB  ALA A  27      51.881  11.779  87.128  1.00  0.76
C
ATOM    153  N   LEU A  28      50.823  10.995  84.231  1.00  0.65           N
ATOM    154  CA  LEU A  28      50.260  10.077  83.260  1.00  0.65
C
ATOM    155  C   LEU A  28      51.119   9.926  81.999  1.00  0.65           C
ATOM    156  O   LEU A  28      51.376   8.819  81.555  1.00  0.65           O
ATOM    157  CB  LEU A  28      48.834  10.527  82.837  1.00  0.65
C
ATOM    158  CG  LEU A  28      48.159   9.632  81.767  1.00  0.65           C
ATOM    159  CD1 LEU A  28      48.022   8.169  82.225  1.00  0.65
C
ATOM    160  CD2 LEU A  28      46.790  10.198  81.360  1.00  0.65
C
ATOM    161  N   SER A  29      51.604  11.053  81.417  1.00  0.73           N
ATOM    162  CA  SER A  29      52.467  11.051  80.232  1.00  0.73
C
ATOM    163  C   SER A  29      53.841  10.443  80.421  1.00  0.73           C
ATOM    164  O   SER A  29      54.351   9.741  79.545  1.00  0.73           O
ATOM    165  CB  SER A  29      52.633  12.446  79.556  1.00  0.73
C
ATOM    166  OG  SER A  29      53.341  13.386  80.367  1.00  0.73
O
ATOM    167  N   LEU A  30      54.508  10.677  81.560  1.00  0.68           N
ATOM    168  CA  LEU A  30      55.768  10.032  81.863  1.00  0.68
C
ATOM    169  C   LEU A  30      55.637   8.528  82.080  1.00  0.68           C
ATOM    170  O   LEU A  30      56.437   7.735  81.601  1.00  0.68           O
ATOM    171  CB  LEU A  30      56.359  10.642  83.145  1.00  0.68
C
ATOM    172  CG  LEU A  30      56.887  12.085  83.057  1.00  0.68
C
ATOM    173  CD1 LEU A  30      57.280  12.580  84.459  1.00  0.68
C
ATOM    174  CD2 LEU A  30      58.102  12.179  82.129  1.00  0.68
C
ATOM    175  N   PHE A  31      54.591   8.109  82.824  1.00  0.56           N
ATOM    176  CA  PHE A  31      54.268   6.716  83.038  1.00  0.56           C
ATOM    177  C   PHE A  31      53.857   5.958  81.798  1.00  0.56           C
ATOM    178  O   PHE A  31      54.279   4.828  81.597  1.00  0.56           O
ATOM    179  CB  PHE A  31      53.142   6.568  84.079  1.00  0.56           C
ATOM    180  CG  PHE A  31      53.697   6.814  85.446  1.00  0.56           C
ATOM    181  CD1 PHE A  31      53.214   7.778  86.352  1.00  0.56
C
ATOM    182  CD2 PHE A  31      54.655   5.897  85.891  1.00  0.56
C
ATOM    183  CE1 PHE A  31      53.625   7.748  87.689  1.00  0.56
C
ATOM    184  CE2 PHE A  31      55.112   5.898  87.204  1.00  0.56
C
ATOM    185  CZ  PHE A  31      54.539   6.773  88.117  1.00  0.56           C
ATOM    186  N   SER A  32      53.043   6.581  80.923  1.00  0.58           N
ATOM    187  CA  SER A  32      52.675   6.031  79.624  1.00  0.58           C
ATOM    188  C   SER A  32      53.883   5.840  78.713  1.00  0.58           C
ATOM    189  O   SER A  32      53.973   4.864  77.970  1.00  0.58           O
ATOM    190  CB  SER A  32      51.593   6.879  78.893  1.00  0.58           C
ATOM    191  OG  SER A  32      52.083   8.140  78.441  1.00  0.58           O
ATOM    192  N   GLY A  33      54.868   6.768  78.785  1.00  0.59           N
ATOM    193  CA  GLY A  33      56.139   6.684  78.075  1.00  0.59
C
ATOM    194  C   GLY A  33      57.054   5.566  78.518  1.00  0.59           C
ATOM    195  O   GLY A  33      57.912   5.142  77.752  1.00  0.59           O
ATOM    196  N   ALA A  34      56.891   5.052  79.758  1.00  0.53           N
ATOM    197  CA  ALA A  34      57.588   3.872  80.257  1.00  0.53
C
ATOM    198  C   ALA A  34      57.219   2.552  79.576  1.00  0.53           C
ATOM    199  O   ALA A  34      58.073   1.679  79.479  1.00  0.53           O
ATOM    200  CB  ALA A  34      57.342   3.626  81.752  1.00  0.53
C
ATOM    201  N   PHE A  35      55.922   2.408  79.180  1.00  0.25           N
ATOM    202  CA  PHE A  35      55.290   1.359  78.371  1.00  0.25           C
ATOM    203  C   PHE A  35      54.085   0.746  79.061  1.00  0.25           C
ATOM    204  O   PHE A  35      53.243   1.456  79.571  1.00  0.25           O
ATOM    205  CB  PHE A  35      56.221   0.305  77.694  1.00  0.25           C
ATOM    206  CG  PHE A  35      57.114   0.927  76.652  1.00  0.25           C
ATOM    207  CD1 PHE A  35      56.986   2.245  76.161  1.00  0.25
C
ATOM    208  CD2 PHE A  35      58.178   0.143  76.189  1.00  0.25
C
ATOM    209  CE1 PHE A  35      57.917   2.763  75.259  1.00  0.25
C
ATOM    210  CE2 PHE A  35      59.089   0.645  75.254  1.00  0.25
C
ATOM    211  CZ  PHE A  35      58.958   1.959  74.789  1.00  0.25           C
ATOM    212  N   THR A  36      53.961  -0.604  79.046  1.00  0.21           N
ATOM    213  CA  THR A  36      52.921  -1.440  79.663  1.00  0.21
C
ATOM    214  C   THR A  36      52.868  -1.382  81.177  1.00  0.21           C
ATOM    215  O   THR A  36      52.013  -1.997  81.808  1.00  0.21           O
ATOM    216  CB  THR A  36      53.069  -2.911  79.255  1.00  0.21
C
ATOM    217  OG1 THR A  36      54.395  -3.383  79.444  1.00  0.21
O
ATOM    218  CG2 THR A  36      52.802  -3.043  77.751  1.00  0.21
C
ATOM    219  N   ALA A  37      53.777  -0.617  81.795  1.00  0.36           N
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ATOM    220  CA  ALA A  37      53.704  -0.221  83.167  1.00  0.36
C
ATOM    221  C   ALA A  37      52.986   1.096  83.307  1.00  0.36           C
ATOM    222  O   ALA A  37      52.620   1.765  82.354  1.00  0.36           O
ATOM    223  CB  ALA A  37      55.123  -0.125  83.720  1.00  0.36
C
ATOM    224  N   ALA A  38      52.715   1.500  84.545  1.00  0.50           N
ATOM    225  CA  ALA A  38      51.921   2.660  84.722  1.00  0.50
C
ATOM    226  C   ALA A  38      52.259   3.201  86.059  1.00  0.50           C
ATOM    227  O   ALA A  38      52.957   2.589  86.875  1.00  0.50           O
ATOM    228  CB  ALA A  38      50.416   2.311  84.676  1.00  0.50
C
ATOM    229  N   GLY A  39      51.739   4.395  86.287  1.00  0.64           N
ATOM    230  CA  GLY A  39      51.710   4.992  87.571  1.00  0.64
C
ATOM    231  C   GLY A  39      50.335   5.278  87.915  1.00  0.64           C
ATOM    232  O   GLY A  39      49.408   5.155  87.119  1.00  0.64           O
ATOM    233  N   GLY A  40      50.209   5.718  89.153  1.00  0.72           N
ATOM    234  CA  GLY A  40      48.942   6.037  89.715  1.00  0.72
C
ATOM    235  C   GLY A  40      48.622   7.485  89.613  1.00  0.72           C
ATOM    236  O   GLY A  40      49.307   8.288  88.987  1.00  0.72           O
ATOM    237  N   ILE A  41      47.551   7.857  90.317  1.00  0.67           N
ATOM    238  CA  ILE A  41      47.192   9.230  90.563  1.00  0.67           C
ATOM    239  C   ILE A  41      48.234   9.849  91.503  1.00  0.67           C
ATOM    240  O   ILE A  41      48.843   9.161  92.311  1.00  0.67           O
ATOM    241  CB  ILE A  41      45.745   9.322  91.060  1.00  0.67           C
ATOM    242  CG1 ILE A  41      44.810   8.828  89.929  1.00  0.67           C
ATOM    243  CG2 ILE A  41      45.391  10.775  91.439  1.00  0.67
C
ATOM    244  CD1 ILE A  41      43.339   8.759  90.353  1.00  0.67           C
ATOM    245  N   MET A  42      48.473  11.172  91.443  1.00  0.71
N
ATOM    246  CA  MET A  42      49.275  11.904  92.403  1.00  0.71
C
ATOM    247  C   MET A  42      48.883  11.688  93.884  1.00  0.71           C
ATOM    248  O   MET A  42      49.724  11.425  94.716  1.00  0.71
O
ATOM    249  CB  MET A  42      49.135  13.396  92.040  1.00  0.71
C
ATOM    250  CG  MET A  42      49.907  14.344  92.970  1.00  0.71
C
ATOM    251  SD  MET A  42      49.661  16.101  92.604  1.00  0.71
S
ATOM    252  CE  MET A  42      47.930  16.196  93.153  1.00  0.71
C
ATOM    253  N   ALA A  43      47.564  11.737  94.223  1.00  0.82           N
ATOM    254  CA  ALA A  43      47.029  11.370  95.529  1.00  0.82
C
ATOM    255  C   ALA A  43      47.302   9.913  95.938  1.00  0.82           C
ATOM    256  O   ALA A  43      47.588   9.623  97.091  1.00  0.82           O
ATOM    257  CB  ALA A  43      45.497  11.611  95.583  1.00  0.82
C
ATOM    258  N   LEU A  44      47.211   8.963  94.974  1.00  0.76           N
ATOM    259  CA  LEU A  44      47.524   7.554  95.170  1.00  0.76           C
ATOM    260  C   LEU A  44      48.997   7.314  95.501  1.00  0.76           C
ATOM    261  O   LEU A  44      49.331   6.633  96.475  1.00  0.76           O
ATOM    262  CB  LEU A  44      47.138   6.783  93.873  1.00  0.76           C
ATOM    263  CG  LEU A  44      47.407   5.265  93.878  1.00  0.76           C
ATOM    264  CD1 LEU A  44      46.654   4.564  95.009  1.00  0.76
C
ATOM    265  CD2 LEU A  44      46.993   4.628  92.544  1.00  0.76
C
ATOM    266  N   ILE A  45      49.915   7.935  94.732  1.00  0.74           N
ATOM    267  CA  ILE A  45      51.360   7.914  94.935  1.00  0.74           C
ATOM    268  C   ILE A  45      51.768   8.583  96.231  1.00  0.74           C
ATOM    269  O   ILE A  45      52.615   8.084  96.972  1.00  0.74           O
ATOM    270  CB  ILE A  45      52.083   8.506  93.731  1.00  0.74           C
ATOM    271  CG1 ILE A  45      52.000   7.467  92.592  1.00  0.74           C
ATOM    272  CG2 ILE A  45      53.559   8.820  94.065  1.00  0.74           C
ATOM    273  CD1 ILE A  45      52.629   7.954  91.285  1.00  0.74           C
ATOM    274  N   LYS A  46      51.131   9.718  96.567  1.00  0.77           N
ATOM    275  CA  LYS A  46      51.326  10.393  97.833  1.00  0.77
C
ATOM    276  C   LYS A  46      50.996   9.538  99.045  1.00  0.77           C
ATOM    277  O   LYS A  46      51.747   9.511 100.016  1.00  0.77           O
ATOM    278  CB  LYS A  46      50.412  11.641  97.924  1.00  0.77
C
ATOM    279  CG  LYS A  46      51.017  12.911  97.307  1.00  0.77
C
ATOM    280  CD  LYS A  46      50.327  14.217  97.745  1.00  0.77
C
ATOM    281  CE  LYS A  46      50.396  14.475  99.260  1.00  0.77
C
ATOM    282  NZ  LYS A  46      49.375  15.460  99.678  1.00  0.77
N
ATOM    283  N   LYS A  47      49.863   8.817  99.003  1.00  0.78           N
ATOM    284  CA  LYS A  47      49.424   7.889 100.025  1.00  0.78
C
ATOM    285  C   LYS A  47      50.364   6.719 100.194  1.00  0.78           C
ATOM    286  O   LYS A  47      50.646   6.253 101.303  1.00  0.78           O
ATOM    287  CB  LYS A  47      48.025   7.392  99.620  1.00  0.78           C
ATOM    288  CG  LYS A  47      47.292   6.576 100.700  1.00  0.78
C
ATOM    289  CD  LYS A  47      45.809   6.313 100.364  1.00  0.78
C
ATOM    290  CE  LYS A  47      45.063   7.584  99.932  1.00  0.78           C
ATOM    291  NZ  LYS A  47      43.647   7.300  99.631  1.00  0.78           N
ATOM    292  N   TYR A  48      50.913   6.219  99.080  1.00  0.71           N
ATOM    293  CA  TYR A  48      51.967   5.235  99.110  1.00  0.71
C
ATOM    294  C   TYR A  48      53.268   5.708  99.736  1.00  0.71           C
ATOM    295  O   TYR A  48      53.894   4.956 100.480  1.00  0.71           O
ATOM    296  CB  TYR A  48      52.280   4.683  97.705  1.00  0.71           C
ATOM    297  CG  TYR A  48      51.162   3.906  97.072  1.00  0.71
C
ATOM    298  CD1 TYR A  48      50.267   3.135  97.835  1.00  0.71
C
ATOM    299  CD2 TYR A  48      51.070   3.857  95.669  1.00  0.71
C
ATOM    300  CE1 TYR A  48      49.307   2.335  97.211  1.00  0.71
C
ATOM    301  CE2 TYR A  48      50.112   3.044  95.043  1.00  0.71
C
ATOM    302  CZ  TYR A  48      49.242   2.275  95.823  1.00  0.71           C
ATOM    303  OH  TYR A  48      48.290   1.419  95.244  1.00  0.71
O
ATOM    304  N   ALA A  49      53.698   6.960  99.478  1.00  0.74           N
ATOM    305  CA  ALA A  49      54.813   7.575 100.167  1.00  0.74
C
ATOM    306  C   ALA A  49      54.588   7.752 101.667  1.00  0.74           C
ATOM    307  O   ALA A  49      55.498   7.505 102.459  1.00  0.74           O
ATOM    308  CB  ALA A  49      55.111   8.954  99.551  1.00  0.74
C
ATOM    309  N   GLN A  50      53.368   8.155 102.090  1.00  0.67           N
ATOM    310  CA  GLN A  50      52.955   8.253 103.485  1.00  0.67
C
ATOM    311  C   GLN A  50      52.993   6.924 104.220  1.00  0.67           C
ATOM    312  O   GLN A  50      53.411   6.852 105.371  1.00  0.67           O
ATOM    313  CB  GLN A  50      51.517   8.825 103.606  1.00  0.67
C
ATOM    314  CG  GLN A  50      51.437  10.315 103.211  1.00  0.67
C
ATOM    315  CD  GLN A  50      49.998  10.825 103.193  1.00  0.67
C
ATOM    316  OE1 GLN A  50      49.017  10.112 103.002  1.00  0.67
O
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ATOM    317  NE2 GLN A  50      49.853  12.159 103.389  1.00  0.67
N
ATOM    318  N   LYS A  51      52.542   5.838 103.561  1.00  0.68           N
ATOM    319  CA  LYS A  51      52.606   4.493 104.088  1.00  0.68
C
ATOM    320  C   LYS A  51      54.006   3.883 104.168  1.00  0.68           C
ATOM    321  O   LYS A  51      54.330   3.197 105.126  1.00  0.68           O
ATOM    322  CB  LYS A  51      51.735   3.565 103.203  1.00  0.68
C
ATOM    323  CG  LYS A  51      51.679   2.097 103.667  1.00  0.68
C
ATOM    324  CD  LYS A  51      50.889   1.227 102.681  1.00  0.68
C
ATOM    325  CE  LYS A  51      51.035  -0.274 102.952  1.00  0.68
C
ATOM    326  NZ  LYS A  51      50.202  -1.048 102.002  1.00  0.68
N
ATOM    327  N   LYS A  52      54.840   4.051 103.111  1.00  0.59           N
ATOM    328  CA  LYS A  52      56.038   3.237 102.967  1.00  0.59
C
ATOM    329  C   LYS A  52      57.366   3.966 102.913  1.00  0.59           C
ATOM    330  O   LYS A  52      58.401   3.331 102.983  1.00  0.59           O
ATOM    331  CB  LYS A  52      56.009   2.502 101.618  1.00  0.59
C
ATOM    332  CG  LYS A  52      54.809   1.581 101.437  1.00  0.59
C
ATOM    333  CD  LYS A  52      54.988   0.831 100.116  1.00  0.59
C
ATOM    334  CE  LYS A  52      53.793  -0.033  99.745  1.00  0.59           C
ATOM    335  NZ  LYS A  52      54.044  -0.692  98.445  1.00  0.59           N
ATOM    336  N   LEU A  53      57.356   5.309 102.747  1.00  0.58           N
ATOM    337  CA  LEU A  53      58.532   6.103 102.428  1.00  0.58
C
ATOM    338  C   LEU A  53      58.871   6.111 100.946  1.00  0.58           C
ATOM    339  O   LEU A  53      58.518   5.212 100.169  1.00  0.58           O
ATOM    340  CB  LEU A  53      59.812   5.828 103.272  1.00  0.58
C
ATOM    341  CG  LEU A  53      59.555   5.813 104.787  1.00  0.58
C
ATOM    342  CD1 LEU A  53      60.669   5.035 105.502  1.00  0.58
C
ATOM    343  CD2 LEU A  53      59.383   7.241 105.320  1.00  0.58
C
ATOM    344  N   TRP A  54      59.570   7.164 100.485  1.00  0.53           N
ATOM    345  CA  TRP A  54      59.947   7.353  99.094  1.00  0.53           C
ATOM    346  C   TRP A  54      60.831   6.265  98.513  1.00  0.53           C
ATOM    347  O   TRP A  54      60.608   5.822  97.392  1.00  0.53           O
ATOM    348  CB  TRP A  54      60.641   8.721  98.895  1.00  0.53           C
ATOM    349  CG  TRP A  54      59.720   9.911  99.042  1.00  0.53           C
ATOM    350  CD1 TRP A  54      58.364   9.981  98.895  1.00  0.53
C
ATOM    351  CD2 TRP A  54      60.166  11.251  99.300  1.00  0.53
C
ATOM    352  NE1 TRP A  54      57.923  11.273  99.083  1.00  0.53
N
ATOM    353  CE2 TRP A  54      59.023  12.068  99.323  1.00  0.53
C
ATOM    354  CE3 TRP A  54      61.440  11.776  99.494  1.00  0.53
C
ATOM    355  CZ2 TRP A  54      59.127  13.435  99.550  1.00  0.53
C
ATOM    356  CZ3 TRP A  54      61.547  13.156  99.721  1.00  0.53
C
ATOM    357  CH2 TRP A  54      60.408  13.974  99.750  1.00  0.53
C
ATOM    358  N   LYS A  55      61.835   5.777  99.272  1.00  0.57           N
ATOM    359  CA  LYS A  55      62.707   4.699  98.836  1.00  0.57           C
ATOM    360  C   LYS A  55      61.979   3.386  98.559  1.00  0.57           C
ATOM    361  O   LYS A  55      62.249   2.718  97.569  1.00  0.57           O
ATOM    362  CB  LYS A  55      63.810   4.428  99.894  1.00  0.57           C
ATOM    363  CG  LYS A  55      64.816   3.346  99.456  1.00  0.57           C
ATOM    364  CD  LYS A  55      65.917   3.102 100.499  1.00  0.57
C
ATOM    365  CE  LYS A  55      66.899   1.998 100.082  1.00  0.57
C
ATOM    366  NZ  LYS A  55      67.942   1.808 101.119  1.00  0.57
N
ATOM    367  N   GLN A  56      61.032   2.992  99.441  1.00  0.54           N
ATOM    368  CA  GLN A  56      60.242   1.786  99.268  1.00  0.54
C
ATOM    369  C   GLN A  56      59.147   1.922  98.234  1.00  0.54           C
ATOM    370  O   GLN A  56      58.703   0.930  97.674  1.00  0.54           O
ATOM    371  CB  GLN A  56      59.550   1.390 100.587  1.00  0.54
C
ATOM    372  CG  GLN A  56      60.522   0.897 101.674  1.00  0.54
C
ATOM    373  CD  GLN A  56      59.754   0.433 102.914  1.00  0.54
C
ATOM    374  OE1 GLN A  56      58.540   0.264 102.932  1.00  0.54
O
ATOM    375  NE2 GLN A  56      60.521   0.162 103.997  1.00  0.54
N
ATOM    376  N   LEU A  57      58.656   3.146  97.965  1.00  0.60           N
ATOM    377  CA  LEU A  57      57.790   3.388  96.835  1.00  0.60           C
ATOM    378  C   LEU A  57      58.458   3.335  95.451  1.00  0.60           C
ATOM    379  O   LEU A  57      57.852   2.946  94.470  1.00  0.60           O
ATOM    380  CB  LEU A  57      57.112   4.752  97.000  1.00  0.60           C
ATOM    381  CG  LEU A  57      56.175   5.076  95.832  1.00  0.60           C
ATOM    382  CD1 LEU A  57      55.100   4.006  95.583  1.00  0.60
C
ATOM    383  CD2 LEU A  57      55.490   6.397  96.091  1.00  0.60
C
ATOM    384  N   ILE A  58      59.721   3.806  95.345  1.00  0.62           N
ATOM    385  CA  ILE A  58      60.557   3.620  94.160  1.00  0.62           C
ATOM    386  C   ILE A  58      60.890   2.152  93.878  1.00  0.62           C
ATOM    387  O   ILE A  58      60.998   1.754  92.726  1.00  0.62           O
ATOM    388  CB  ILE A  58      61.857   4.426  94.277  1.00  0.62           C
ATOM    389  CG1 ILE A  58      61.549   5.943  94.235  1.00  0.62           C
ATOM    390  CG2 ILE A  58      62.871   4.041  93.163  1.00  0.62           C
ATOM    391  CD1 ILE A  58      62.751   6.802  94.657  1.00  0.62           C
ATOM    392  N   ALA A  59      61.122   1.367  94.954  1.00  0.66           N
ATOM    393  CA  ALA A  59      61.358  -0.061  94.896  1.00  0.66
C
ATOM    394  C   ALA A  59      60.155  -0.963  94.467  1.00  0.66           C
ATOM    395  O   ALA A  59      59.002  -0.484  94.308  1.00  0.66           O
ATOM    396  CB  ALA A  59      61.852  -0.531  96.286  1.00  0.66
C
ATOM    397  OXT ALA A  59      60.413  -2.189  94.290  1.00  0.66
O
TER     398      ALA A  59
END
```

B)

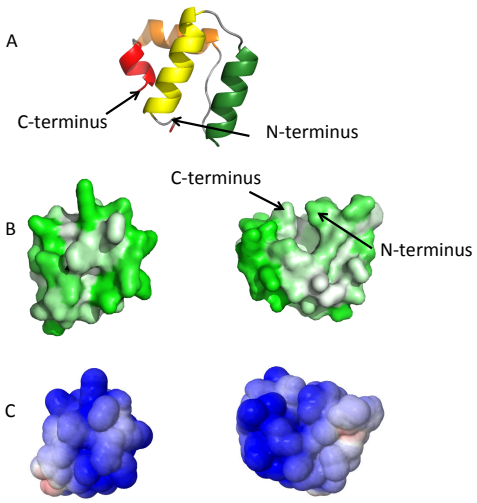

Figure S5- Structural models of garvacin ML. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of garvacin ML. Orientation peptide backbone in surface filling diagrams, B and C, correlate to one another.

6.Mutacin BhtB

A) PDB file for model of Mutacin BhtB. Structure modeled after lacticin Q using SWISS-MODEL[84]

TITLE SWISS-MODEL SERVER (https://swissmodel.expasy.org)
TITLE 2 Untitled Project
EXPDTA THEORETICAL MODEL (SWISS-MODEL SERVER)
AUTHOR SWISS-MODEL SERVER (SEE REFERENCE IN JRNL Records)
REVDAT 1 15-AUG-16 1MOD 1 21:39
JRNL AUTH
M.BIASINI,S.BIENERT,A.WATERHOUSE,K.ARNOLD,G.STUDER,
JRNL AUTH 2 T.SCHMIDT,F.KIEFER,T.GALLO
CASSARINO,M.BERTONI,L.BORDOLI,
JRNL AUTH 3 T.SCHWEDE
JRNL TITL SWISS-MODEL: MODELLING PROTEIN TERTIARY AND QUATERNARY
JRNL TITL 2 STRUCTURE USING EVOLUTIONARY INFORMATION
JRNL REF NUCLEIC.ACIDS.RES 2014
JRNL REFN ISSN 0305-1048
JRNL PMID 24782522
JRNL DOI 10.1093/nar/gku340
REMARK 3
REMARK 3 MODEL INFORMATION
REMARK 3 ENGIN PROMOD3
REMARK 3 VERSN 1.0.0
REMARK 3 OSTAT MONOMER
REMARK 3 OSRSN USER
REMARK 3 GMQE 0.74
REMARK 3 QMN4 -1.71
REMARK 3
REMARK 3 TEMPLATE 1
REMARK 3 PDBID 2n8p
REMARK 3 CHAIN A
REMARK 3 MMCIF A
REMARK 3 PDBV 2016-08-12
REMARK 3 SMTLE 2n8p.1.A
REMARK 3 SMTLV 2016-08-14
REMARK 3 MTHD SOLUTION NMR 0.00 A
REMARK 3 FOUND HHblits
REMARK 3 GMQE 0.74
REMARK 3 SIM 0.43
REMARK 3 SID 45.24
REMARK 3 OSTAT monomer
ATOM 1 N TRP A 2 9.109 -0.818 -0.130 1.00 0.48 N
ATOM 2 CA TRP A 2 10.436 -1.289 -0.665 1.00 0.48 C
ATOM 3 C TRP A 2 10.867 -0.538 -1.927 1.00 0.48 C
ATOM 4 O TRP A 2 11.803 0.265 -1.816 1.00 0.48 O
ATOM 5 CB TRP A 2 10.478 -2.840 -0.737 1.00 0.48 C
ATOM 6 CG TRP A 2 11.868 -3.431 -0.982 1.00 0.48 C
ATOM 7 CD1 TRP A 2 13.012 -3.412 -0.217 1.00 0.48 C
ATOM 8 CD2 TRP A 2 12.196 -4.175 -2.166 1.00 0.48 C
ATOM 9 NE1 TRP A 2 14.021 -4.105 -0.853 1.00 0.48 N
ATOM 10 CE2 TRP A 2 13.539 -4.578 -2.042 1.00 0.48 C
ATOM 11 CE3 TRP A 2 11.445 -4.512 -3.289 1.00 0.48 C
ATOM 12 CZ2 TRP A 2 14.154 -5.326 -3.029 1.00 0.48 C
ATOM 13 CZ3 TRP A 2 12.069 -5.276 -4.285 1.00 0.48 C
ATOM 14 CH2 TRP A 2 13.401 -5.686 -4.152 1.00 0.48 C
ATOM 15 N GLY A 3 10.233 -0.618 -3.127 1.00 0.61 N
ATOM 16 CA GLY A 3 10.771 0.129 -4.291 1.00 0.61 C
ATOM 17 C GLY A 3 10.911 1.649 -4.148 1.00 0.61 C

```
ATOM     18  O   GLY A   3      11.784   2.266  -4.752  1.00  0.61           O
ATOM     19  N   ARG A   4      10.071   2.287  -3.310  1.00  0.50           N
ATOM     20  CA  ARG A   4      10.164   3.700  -2.950  1.00  0.50           C
ATOM     21  C   ARG A   4      11.385   4.114  -2.117  1.00  0.50           C
ATOM     22  O   ARG A   4      12.016   5.130  -2.400  1.00  0.50           O
ATOM     23  CB  ARG A   4       8.886   4.147  -2.206  1.00  0.50           C
ATOM     24  CG  ARG A   4       7.603   4.020  -3.050  1.00  0.50           C
ATOM     25  CD  ARG A   4       6.366   4.465  -2.267  1.00  0.50           C
ATOM     26  NE  ARG A   4       5.188   4.302  -3.177  1.00  0.50           N
ATOM     27  CZ  ARG A   4       3.915   4.473  -2.793  1.00  0.50           C
ATOM     28  NH1 ARG A   4       2.934   4.351  -3.685  1.00  0.50           N
ATOM     29  NH2 ARG A   4       3.595   4.782  -1.540  1.00  0.50           N
ATOM     30  N   ILE A   5      11.775   3.335  -1.078  1.00  0.51           N
ATOM     31  CA  ILE A   5      12.965   3.591  -0.259  1.00  0.51           C
ATOM     32  C   ILE A   5      14.237   3.498  -1.117  1.00  0.51           C
ATOM     33  O   ILE A   5      15.189   4.260  -0.935  1.00  0.51           O
ATOM     34  CB  ILE A   5      13.024   2.749   1.041  1.00  0.51           C
ATOM     35  CG1 ILE A   5      13.102   1.232   0.764  1.00  0.51           C
ATOM     36  CG2 ILE A   5      11.783   3.082   1.903  1.00  0.51           C
ATOM     37  CD1 ILE A   5      13.354   0.308   1.964  1.00  0.51           C
ATOM     38  N   LEU A   6      14.247   2.584  -2.117  1.00  0.57           N
ATOM     39  CA  LEU A   6      15.290   2.390  -3.126  1.00  0.57           C
ATOM     40  C   LEU A   6      15.480   3.511  -4.097  1.00  0.57           C
ATOM     41  O   LEU A   6      16.590   3.791  -4.550  1.00  0.57           O
ATOM     42  CB  LEU A   6      15.022   1.125  -3.979  1.00  0.57           C
ATOM     43  CG  LEU A   6      14.952  -0.125  -3.084  1.00  0.57           C
ATOM     44  CD1 LEU A   6      14.763  -1.459  -3.808  1.00  0.57           C
ATOM     45  CD2 LEU A   6      16.263  -0.231  -2.295  1.00  0.57           C
ATOM     46  N   ALA A   7      14.371   4.158  -4.468  1.00  0.62           N
ATOM     47  CA  ALA A   7      14.361   5.222  -5.432  1.00  0.62           C
ATOM     48  C   ALA A   7      15.186   6.408  -4.954  1.00  0.62           C
ATOM     49  O   ALA A   7      15.955   7.003  -5.708  1.00  0.62           O
ATOM     50  CB  ALA A   7      12.900   5.608  -5.715  1.00  0.62           C
ATOM     51  N   PHE A   8      15.104   6.727  -3.649  1.00  0.47           N
ATOM     52  CA  PHE A   8      15.924   7.737  -3.007  1.00  0.47           C
ATOM     53  C   PHE A   8      17.401   7.441  -3.022  1.00  0.47           C
ATOM     54  O   PHE A   8      18.222   8.349  -3.121  1.00  0.47           O
ATOM     55  CB  PHE A   8      15.532   7.923  -1.532  1.00  0.47           C
ATOM     56  CG  PHE A   8      14.181   8.544  -1.440  1.00  0.47           C
ATOM     57  CD1 PHE A   8      13.147   7.912  -0.736  1.00  0.47           C
ATOM     58  CD2 PHE A   8      13.943   9.787  -2.045  1.00  0.47           C
ATOM     59  CE1 PHE A   8      11.892   8.522  -0.627  1.00  0.47           C
ATOM     60  CE2 PHE A   8      12.684  10.387  -1.960  1.00  0.47           C
ATOM     61  CZ  PHE A   8      11.658   9.759  -1.243  1.00  0.47           C
ATOM     62  N   VAL A   9      17.787   6.161  -2.926  1.00  0.56           N
ATOM     63  CA  VAL A   9      19.167   5.734  -2.966  1.00  0.56           C
ATOM     64  C   VAL A   9      19.878   6.103  -4.274  1.00  0.56           C
ATOM     65  O   VAL A   9      21.082   6.353  -4.276  1.00  0.56           O
ATOM     66  CB  VAL A   9      19.328   4.249  -2.672  1.00  0.56           C
ATOM     67  CG1 VAL A   9      20.830   3.966  -2.514  1.00  0.56           C
ATOM     68  CG2 VAL A   9      18.719   3.841  -1.318  1.00  0.56           C
ATOM     69  N   ALA A  10      19.143   6.240  -5.403  1.00  0.54           N
ATOM     70  CA  ALA A  10      19.645   6.697  -6.693  1.00  0.54           C
ATOM     71  C   ALA A  10      20.451   8.006  -6.636  1.00  0.54           C
ATOM     72  O   ALA A  10      21.399   8.203  -7.398  1.00  0.54           O
ATOM     73  CB  ALA A  10      18.434   6.861  -7.638  1.00  0.54           C
ATOM     74  N   LYS A  11      20.115   8.909  -5.685  1.00  0.44           N
ATOM     75  CA  LYS A  11      20.882  10.098  -5.339  1.00  0.44           C
ATOM     76  C   LYS A  11      22.294   9.832  -4.785  1.00  0.44           C
ATOM     77  O   LYS A  11      23.212  10.621  -5.011  1.00  0.44           O
ATOM     78  CB  LYS A  11      20.067  11.015  -4.365  1.00  0.44           C
ATOM     79  CG  LYS A  11      20.105  10.641  -2.865  1.00  0.44           C
ATOM     80  CD  LYS A  11      21.217  11.330  -2.061  1.00  0.44           C
ATOM     81  CE  LYS A  11      20.772  12.643  -1.427  1.00  0.44           C
ATOM     82  NZ  LYS A  11      21.970  13.473  -1.207  1.00  0.44           N
ATOM     83  N   TYR A  12      22.475   8.751  -3.984  1.00  0.39           N
ATOM     84  CA  TYR A  12      23.710   8.330  -3.324  1.00  0.39           C
ATOM     85  C   TYR A  12      24.642   7.672  -4.320  1.00  0.39           C
ATOM     86  O   TYR A  12      25.863   7.790  -4.232  1.00  0.39           O
ATOM     87  CB  TYR A  12      23.455   7.337  -2.141  1.00  0.39           C
ATOM     88  CG  TYR A  12      23.015   8.036  -0.877  1.00  0.39           C
ATOM     89  CD1 TYR A  12      23.974   8.677  -0.076  1.00  0.39           C
ATOM     90  CD2 TYR A  12      21.682   8.004  -0.430  1.00  0.39           C
ATOM     91  CE1 TYR A  12      23.611   9.291   1.134  1.00  0.39           C
ATOM     92  CE2 TYR A  12      21.317   8.613   0.780  1.00  0.39           C
ATOM     93  CZ  TYR A  12      22.278   9.261   1.563  1.00  0.39           C
ATOM     94  OH  TYR A  12      21.865   9.852   2.781  1.00  0.39           O
ATOM     95  N   GLY A  13      24.070   6.953  -5.300  1.00  0.49           N
ATOM     96  CA  GLY A  13      24.817   6.346  -6.382  1.00  0.49           C
ATOM     97  C   GLY A  13      24.294   4.964  -6.655  1.00  0.49           C
ATOM     98  O   GLY A  13      23.115   4.661  -6.475  1.00  0.49           O
ATOM     99  N   THR A  14      25.186   4.062  -7.099  1.00  0.50           N
ATOM    100  CA  THR A  14      24.845   2.709  -7.524  1.00  0.50           C
ATOM    101  C   THR A  14      25.397   1.656  -6.578  1.00  0.50           C
ATOM    102  O   THR A  14      25.439   0.466  -6.893  1.00  0.50           O
ATOM    103  CB  THR A  14      25.283   2.416  -8.952  1.00  0.50           C
ATOM    104  OG1 THR A  14      26.642   2.772  -9.177  1.00  0.50
O
ATOM    105  CG2 THR A  14      24.415   3.294  -9.866  1.00  0.50
C
ATOM    106  N   LYS A  15      25.802   2.054  -5.351  1.00  0.52           N
ATOM    107  CA  LYS A  15      26.430   1.147  -4.401  1.00  0.52           C
ATOM    108  C   LYS A  15      25.547   0.831  -3.208  1.00  0.52           C
ATOM    109  O   LYS A  15      25.326  -0.330  -2.869  1.00  0.52           O
ATOM    110  CB  LYS A  15      27.757   1.772  -3.925  1.00  0.52           C
ATOM    111  CG  LYS A  15      28.673   0.818  -3.142  1.00  0.52           C
ATOM    112  CD  LYS A  15      30.101   1.388  -3.047  1.00  0.52           C
ATOM    113  CE  LYS A  15      30.957   1.247  -4.315  1.00  0.52           C
ATOM    114  NZ  LYS A  15      31.339  -0.168  -4.519  1.00  0.52           N
ATOM    115  N   ALA A  16      24.944   1.854  -2.573  1.00  0.63           N
ATOM    116  CA  ALA A  16      24.040   1.666  -1.459  1.00  0.63           C
ATOM    117  C   ALA A  16      22.711   1.028  -1.901  1.00  0.63           C
ATOM    118  O   ALA A  16      22.036   0.348  -1.126  1.00  0.63           O
ATOM    119  CB  ALA A  16      23.857   3.039  -0.772  1.00  0.63           C
ATOM    120  N   VAL A  17      22.329   1.203  -3.195  1.00  0.61           N
ATOM    121  CA  VAL A  17      21.102   0.706  -3.818  1.00  0.61           C
ATOM    122  C   VAL A  17      21.126  -0.804  -3.874  1.00  0.61           C
ATOM    123  O   VAL A  17      20.144  -1.495  -3.600  1.00  0.61           O
ATOM    124  CB  VAL A  17      20.829   1.371  -5.185  1.00  0.61           C
ATOM    125  CG1 VAL A  17      21.903   1.094  -6.259  1.00  0.61
C
ATOM    126  CG2 VAL A  17      19.402   1.073  -5.697  1.00  0.61
C
ATOM    127  N   GLN A  18      22.321  -1.352  -4.159  1.00  0.62           N
ATOM    128  CA  GLN A  18      22.577  -2.764  -4.288  1.00  0.62           C
ATOM    129  C   GLN A  18      22.314  -3.540  -3.009  1.00  0.62           C
ATOM    130  O   GLN A  18      21.824  -4.672  -3.036  1.00  0.62           O
ATOM    131  CB  GLN A  18      24.020  -2.980  -4.779  1.00  0.62           C
ATOM    132  CG  GLN A  18      24.221  -4.434  -5.239  1.00  0.62           C
ATOM    133  CD  GLN A  18      25.457  -4.562  -6.112  1.00  0.62           C
ATOM    134  OE1 GLN A  18      26.551  -4.904  -5.647  1.00  0.62
O
ATOM    135  NE2 GLN A  18      25.292  -4.273  -7.419  1.00  0.62
N
ATOM    136  N   TRP A  19      22.611  -2.933  -1.846  1.00  0.52           N
ATOM    137  CA  TRP A  19      22.476  -3.547  -0.537  1.00  0.52           C
ATOM    138  C   TRP A  19      21.049  -3.965  -0.218  1.00  0.52           C
ATOM    139  O   TRP A  19      20.787  -5.048   0.341  1.00  0.52           O
ATOM    140  CB  TRP A  19      22.911  -2.541   0.563  1.00  0.52           C
ATOM    141  CG  TRP A  19      22.915  -3.200   1.929  1.00  0.52           C
ATOM    142  CD1 TRP A  19      23.664  -4.280   2.283  1.00  0.52           C
ATOM    143  CD2 TRP A  19      22.000  -2.969   3.019  1.00  0.52           C
ATOM    144  NE1 TRP A  19      23.296  -4.742   3.524  1.00  0.52           N
ATOM    145  CE2 TRP A  19      22.260  -3.960   3.987  1.00  0.52           C
ATOM    146  CE3 TRP A  19      21.014  -2.006   3.224  1.00  0.52           C
ATOM    147  CZ2 TRP A  19      21.567  -3.992   5.192  1.00  0.52           C
ATOM    148  CZ3 TRP A  19      20.420  -1.957   4.494  1.00  0.52           C
ATOM    149  CH2 TRP A  19      20.698  -2.928   5.466  1.00  0.52           C
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ATOM    150  N   ALA A  20      20.109  -3.072  -0.540  1.00  0.66           N
ATOM    151  CA  ALA A  20      18.705  -3.170  -0.240  1.00  0.66           C
ATOM    152  C   ALA A  20      17.903  -3.900  -1.317  1.00  0.66           C
ATOM    153  O   ALA A  20      16.890  -4.535  -0.995  1.00  0.66           O
ATOM    154  CB  ALA A  20      18.278  -1.686   0.002  1.00  0.66           C
ATOM    155  N   TRP A  21      18.366  -3.900  -2.589  1.00  0.54           N
ATOM    156  CA  TRP A  21      17.972  -4.869  -3.615  1.00  0.54           C
ATOM    157  C   TRP A  21      18.362  -6.303  -3.281  1.00  0.54           C
ATOM    158  O   TRP A  21      17.581  -7.237  -3.471  1.00  0.54           O
ATOM    159  CB  TRP A  21      18.550  -4.554  -5.021  1.00  0.54           C
ATOM    160  CG  TRP A  21      17.697  -3.608  -5.834  1.00  0.54           C
ATOM    161  CD1 TRP A  21      17.895  -2.281  -6.032  1.00  0.54
C
ATOM    162  CD2 TRP A  21      16.498  -3.948  -6.558  1.00  0.54
C
ATOM    163  NE1 TRP A  21      16.907  -1.749  -6.835  1.00  0.54
N
ATOM    164  CE2 TRP A  21      16.031  -2.767  -7.162  1.00  0.54           C
ATOM    165  CE3 TRP A  21      15.822  -5.154  -6.713  1.00  0.54           C
ATOM    166  CZ2 TRP A  21      14.867  -2.764  -7.930  1.00  0.54           C
ATOM    167  CZ3 TRP A  21      14.655  -5.155  -7.490  1.00  0.54           C
ATOM    168  CH2 TRP A  21      14.181  -3.981  -8.088  1.00  0.54
C
ATOM    169  N   LYS A  22      19.599  -6.497  -2.781  1.00  0.65           N
ATOM    170  CA  LYS A  22      20.102  -7.765  -2.290  1.00  0.65           C
ATOM    171  C   LYS A  22      19.352  -8.296  -1.063  1.00  0.65           C
ATOM    172  O   LYS A  22      18.976  -9.467  -1.000  1.00  0.65           O
ATOM    173  CB  LYS A  22      21.606  -7.600  -1.946  1.00  0.65           C
ATOM    174  CG  LYS A  22      22.293  -8.893  -1.493  1.00  0.65           C
ATOM    175  CD  LYS A  22      23.788  -8.701  -1.188  1.00  0.65           C
ATOM    176  CE  LYS A  22      24.453  -9.998  -0.716  1.00  0.65           C
ATOM    177  NZ  LYS A  22      25.895  -9.790  -0.453  1.00  0.65           N
ATOM    178  N   ASN A  23      19.098  -7.430  -0.058  1.00  0.64           N
ATOM    179  CA  ASN A  23      18.428  -7.784   1.185  1.00  0.64           C
ATOM    180  C   ASN A  23      16.974  -7.378   1.185  1.00  0.64           C
ATOM    181  O   ASN A  23      16.552  -6.421   1.838  1.00  0.64           O
ATOM    182  CB  ASN A  23      19.086  -7.145   2.422  1.00  0.64           C
ATOM    183  CG  ASN A  23      20.411  -7.840   2.638  1.00  0.64           C
ATOM    184  OD1 ASN A  23      20.442  -9.008   3.049  1.00  0.64
O
ATOM    185  ND2 ASN A  23      21.536  -7.151   2.376  1.00  0.64
N
ATOM    186  N   LYS A  24      16.153  -8.171   0.486  1.00  0.55           N
ATOM    187  CA  LYS A  24      14.736  -7.961   0.349  1.00  0.55           C
ATOM    188  C   LYS A  24      13.943  -8.840   1.299  1.00  0.55           C
ATOM    189  O   LYS A  24      12.953  -9.467   0.920  1.00  0.55           O
ATOM    190  CB  LYS A  24      14.340  -8.221  -1.116  1.00  0.55           C
ATOM    191  CG  LYS A  24      14.686  -9.615  -1.669  1.00  0.55           C
ATOM    192  CD  LYS A  24      14.249  -9.733  -3.139  1.00  0.55           C
ATOM    193  CE  LYS A  24      12.740  -9.851  -3.382  1.00  0.55           C
ATOM    194  NZ  LYS A  24      12.299 -11.222  -3.045  1.00  0.55
N
ATOM    195  N   TRP A  25      14.393  -8.941   2.565  1.00  0.37           N
ATOM    196  CA  TRP A  25      13.669  -9.684   3.576  1.00  0.37           C
ATOM    197  C   TRP A  25      13.757  -9.015   4.949  1.00  0.37           C
ATOM    198  O   TRP A  25      12.754  -8.887   5.648  1.00  0.37           O
ATOM    199  CB  TRP A  25      14.179 -11.158   3.605  1.00  0.37           C
ATOM    200  CG  TRP A  25      15.660 -11.307   3.922  1.00  0.37           C
ATOM    201  CD1 TRP A  25      16.746 -11.214   3.093  1.00  0.37
C
ATOM    202  CD2 TRP A  25      16.183 -11.441   5.255  1.00  0.37
C
ATOM    203  NE1 TRP A  25      17.914 -11.259   3.823  1.00  0.37
N
ATOM    204  CE2 TRP A  25      17.586 -11.407   5.152  1.00  0.37
C
ATOM    205  CE3 TRP A  25      15.549 -11.545   6.492  1.00  0.37
C
ATOM    206  CZ2 TRP A  25      18.387 -11.488   6.284  1.00  0.37
C
ATOM    207  CZ3 TRP A  25      16.357 -11.619   7.634  1.00  0.37
C
ATOM    208  CH2 TRP A  25      17.755 -11.591   7.533  1.00  0.37
C
ATOM    209  N   PHE A  26      14.938  -8.487   5.343  1.00  0.35           N
ATOM    210  CA  PHE A  26      15.150  -7.843   6.634  1.00  0.35           C
ATOM    211  C   PHE A  26      14.695  -6.387   6.621  1.00  0.35           C
ATOM    212  O   PHE A  26      14.257  -5.818   7.617  1.00  0.35           O
ATOM    213  CB  PHE A  26      16.659  -7.970   6.964  1.00  0.35           C
ATOM    214  CG  PHE A  26      16.961  -7.576   8.384  1.00  0.35           C
ATOM    215  CD1 PHE A  26      16.593  -8.393   9.467  1.00  0.35           C
ATOM    216  CD2 PHE A  26      17.574  -6.341   8.641  1.00  0.35           C
ATOM    217  CE1 PHE A  26      16.845  -7.981  10.784  1.00  0.35
C
ATOM    218  CE2 PHE A  26      17.812  -5.921   9.954  1.00  0.35           C
ATOM    219  CZ  PHE A  26      17.455  -6.745  11.027  1.00  0.35           C
ATOM    220  N   LEU A  27      14.732  -5.766   5.434  1.00  0.44           N
ATOM    221  CA  LEU A  27      14.284  -4.406   5.200  1.00  0.44           C
ATOM    222  C   LEU A  27      12.835  -4.377   4.798  1.00  0.44           C
ATOM    223  O   LEU A  27      12.274  -3.294   4.524  1.00  0.44           O
ATOM    224  CB  LEU A  27      15.041  -3.796   4.008  1.00  0.44           C
ATOM    225  CG  LEU A  27      16.561  -3.740   4.163  1.00  0.44           C
ATOM    226  CD1 LEU A  27      17.127  -3.231   2.840  1.00  0.44
C
ATOM    227  CD2 LEU A  27      17.001  -2.850   5.333  1.00  0.44
C
ATOM    228  N   LEU A  28      12.130  -5.510   4.760  1.00  0.39           N
ATOM    229  CA  LEU A  28      10.705  -5.479   4.560  1.00  0.39           C
ATOM    230  C   LEU A  28       9.943  -5.157   5.835  1.00  0.39           C
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C
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ATOM    241  OG  SER A  29      11.754  -6.314   9.471  1.00  0.33           O
ATOM    242  N   LEU A  30      10.827  -2.897   8.117  1.00  0.34           N
ATOM    243  CA  LEU A  30      11.103  -1.516   8.497  1.00  0.34           C
ATOM    244  C   LEU A  30       9.830  -0.735   8.838  1.00  0.34           C
ATOM    245  O   LEU A  30       8.851  -0.743   8.093  1.00  0.34           O
ATOM    246  CB  LEU A  30      11.842  -0.773   7.356  1.00  0.34           C
ATOM    247  CG  LEU A  30      13.233  -1.311   6.948  1.00  0.34           C
ATOM    248  CD1 LEU A  30      13.605  -0.625   5.614  1.00  0.34
C
ATOM    249  CD2 LEU A  30      14.352  -1.428   8.018  1.00  0.34
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ATOM    250  N   GLY A  31       9.814  -0.035   9.996  1.00  0.32           N
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ATOM    252  C   GLY A  31       8.333   1.985   9.885  1.00  0.32           C
ATOM    253  O   GLY A  31       7.291   2.588  10.161  1.00  0.32           O
ATOM    254  N   GLU A  32       9.262   2.491   9.068  1.00  0.32           N
ATOM    255  CA  GLU A  32       9.230   3.774   8.435  1.00  0.32           C
ATOM    256  C   GLU A  32       9.892   3.638   7.073  1.00  0.32           C
ATOM    257  O   GLU A  32      10.245   2.465   6.649  1.00  0.32           O
ATOM    258  CB  GLU A  32       9.899   4.876   9.337  1.00  0.32           C
ATOM    259  CG  GLU A  32      11.354   4.601   9.771  1.00  0.32           C
ATOM    260  CD  GLU A  32      11.900   5.633  10.762  1.00  0.32
C
ATOM    261  OE1 GLU A  32      11.164   6.591  11.109  1.00  0.32
O
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ATOM    262  OE2 GLU A  32      13.071   5.438  11.181  1.00  0.32
O
ATOM    263  N   ALA A  33      10.124   4.671   6.292  1.00  0.46
N
ATOM    264  CA  ALA A  33      11.170   4.770   5.290  1.00  0.46
C
ATOM    265  C   ALA A  33      12.565   4.967   5.911  1.00  0.46
C
ATOM    266  O   ALA A  33      12.788   5.909   6.660  1.00  0.46
O
ATOM    267  CB  ALA A  33      10.897   5.974   4.375  1.00  0.46
C
ATOM    268  N   VAL A  34      13.558   4.096   5.611  1.00  0.45
N
ATOM    269  CA  VAL A  34      14.737   3.968   6.460  1.00  0.45
C
ATOM    270  C   VAL A  34      16.021   4.388   5.850  1.00  0.45
C
ATOM    271  O   VAL A  34      16.373   3.928   4.770  1.00  0.45
O
ATOM    272  CB  VAL A  34      14.852   2.542   6.923  1.00  0.45
C
ATOM    273  CG1 VAL A  34      16.140   2.277   7.768  1.00  0.45
C
ATOM    274  CG2 VAL A  34      13.542   2.441   7.749  1.00  0.45
C
ATOM    275  N   PHE A  35      16.774   5.242   6.582  1.00  0.39
N
ATOM    276  CA  PHE A  35      18.101   5.649   6.155  1.00  0.39
C
ATOM    277  C   PHE A  35      19.093   5.681   7.313  1.00  0.39
C
ATOM    278  O   PHE A  35      20.302   5.479   7.108  1.00  0.39
O
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C
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C
ATOM    281  CD1 PHE A  35      15.949   7.311   4.162  1.00  0.39
C
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C
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C
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C
ATOM    285  CZ  PHE A  35      15.789   6.675   1.832  1.00  0.39
C
ATOM    286  N   ASP A  36      18.640   5.861   8.567  1.00  0.46
N
ATOM    287  CA  ASP A  36      19.470   5.867   9.768  1.00  0.46
C
ATOM    288  C   ASP A  36      20.159   4.529  10.019  1.00  0.46
C
ATOM    289  O   ASP A  36      21.322   4.450  10.422  1.00  0.46
O
ATOM    290  CB  ASP A  36      18.624   6.376  10.965  1.00  0.46
C
ATOM    291  CG  ASP A  36      18.354   7.871  10.786  1.00  0.46
C
ATOM    292  OD1 ASP A  36      18.928   8.478   9.838  1.00  0.46
O
ATOM    293  OD2 ASP A  36      17.586   8.423  11.608  1.00  0.46
O
ATOM    294  N   TYR A  37      19.462   3.436   9.668  1.00  0.35
N
ATOM    295  CA  TYR A  37      19.933   2.067   9.715  1.00  0.35
C
ATOM    296  C   TYR A  37      20.575   1.644   8.387  1.00  0.35
C
ATOM    297  O   TYR A  37      20.548   0.469   8.025  1.00  0.35
O
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C
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C
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C
ATOM    301  CD2 TYR A  37      18.609   0.896  12.517  1.00  0.35
C
ATOM    302  CE1 TYR A  37      16.302   2.466  12.635  1.00  0.35
C
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C
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C
ATOM    305  OH  TYR A  37      16.145   2.115  15.023  1.00  0.35
O
ATOM    306  N   ILE A  38      21.153   2.590   7.606  1.00  0.42
N
ATOM    307  CA  ILE A  38      21.929   2.283   6.402  1.00  0.42
C
ATOM    308  C   ILE A  38      23.346   2.835   6.532  1.00  0.42
C
ATOM    309  O   ILE A  38      24.319   2.165   6.179  1.00  0.42
O
ATOM    310  CB  ILE A  38      21.273   2.835   5.130  1.00  0.42
C
ATOM    311  CG1 ILE A  38      19.838   2.268   4.998  1.00  0.42
C
ATOM    312  CG2 ILE A  38      22.126   2.505   3.878  1.00  0.42
C
ATOM    313  CD1 ILE A  38      19.093   2.723   3.741  1.00  0.42
C
ATOM    314  N   ARG A  39      23.513   4.043   7.122  1.00  0.41
N
ATOM    315  CA  ARG A  39      24.811   4.684   7.331  1.00  0.41
C
ATOM    316  C   ARG A  39      25.681   3.974   8.354  1.00  0.41
C
ATOM    317  O   ARG A  39      26.900   4.132   8.371  1.00  0.41
O
ATOM    318  CB  ARG A  39      24.637   6.134   7.842  1.00  0.41
C
ATOM    319  CG  ARG A  39      23.988   7.096   6.833  1.00  0.41
C
ATOM    320  CD  ARG A  39      23.823   8.498   7.424  1.00  0.41
C
ATOM    321  NE  ARG A  39      23.240   9.355   6.342  1.00  0.41
N
ATOM    322  CZ  ARG A  39      22.824  10.615   6.526  1.00  0.41
C
ATOM    323  NH1 ARG A  39      22.306  11.289   5.499  1.00  0.41
N
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N
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N
ATOM    326  CA  SER A  40      25.818   2.354  10.181  1.00  0.39
C
ATOM    327  C   SER A  40      26.104   0.959   9.643  1.00  0.39
C
ATOM    328  O   SER A  40      26.960   0.258  10.182  1.00  0.39
O
ATOM    329  CB  SER A  40      25.012   2.194  11.496  1.00  0.39
C
ATOM    330  OG  SER A  40      23.705   1.666  11.235  1.00  0.39
O
ATOM    331  N   ILE A  41      25.409   0.520   8.570  1.00  0.38
N
ATOM    332  CA  ILE A  41      25.596  -0.808   7.995  1.00  0.38
C
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C
ATOM    334  O   ILE A  41      27.652  -1.589   7.039  1.00  0.38
O
ATOM    335  CB  ILE A  41      24.311  -1.302   7.321  1.00  0.38
C
ATOM    336  CG1 ILE A  41      23.103  -1.350   8.293  1.00  0.38
C
ATOM    337  CG2 ILE A  41      24.545  -2.659   6.610  1.00  0.38
C
ATOM    338  CD1 ILE A  41      23.220  -2.304   9.488  1.00  0.38
C
ATOM    339  N   TRP A  42      26.562  -0.009   5.867  1.00  0.31
N
ATOM    340  CA  TRP A  42      27.550   0.015   4.805  1.00  0.31
C
ATOM    341  C   TRP A  42      28.626   1.046   5.136  1.00  0.31
C
ATOM    342  O   TRP A  42      29.814   0.727   5.205  1.00  0.31
O
ATOM    343  CB  TRP A  42      26.831   0.302   3.452  1.00  0.31
C
ATOM    344  CG  TRP A  42      27.743   0.380   2.238  1.00  0.31
C
ATOM    345  CD1 TRP A  42      28.333   1.488   1.700  1.00  0.31
C
ATOM    346  CD2 TRP A  42      28.278  -0.748   1.529  1.00  0.31
C
ATOM    347  NE1 TRP A  42      29.201   1.134   0.685  1.00  0.31
N
ATOM    348  CE2 TRP A  42      29.198  -0.248   0.587  1.00  0.31
C
ATOM    349  CE3 TRP A  42      28.072  -2.116   1.682  1.00  0.31
C
ATOM    350  CZ2 TRP A  42      29.928  -1.114  -0.222  1.00  0.31
C
ATOM    351  CZ3 TRP A  42      28.766  -2.983   0.829  1.00  0.31
C
ATOM    352  CH2 TRP A  42      29.677  -2.493  -0.114  1.00  0.31
C
ATOM    353  N   GLY A  43      28.196   2.294   5.397  1.00  0.42
N
ATOM    354  CA  GLY A  43      29.042   3.445   5.670  1.00  0.42
C
ATOM    355  C   GLY A  43      28.745   4.566   4.655  1.00  0.42
C
ATOM    356  O   GLY A  43      27.815   4.395   3.814  1.00  0.42
O
ATOM    357  OXT GLY A  43      29.431   5.621   4.728  1.00  0.42
O
TER     358      GLY A  43
END
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B)

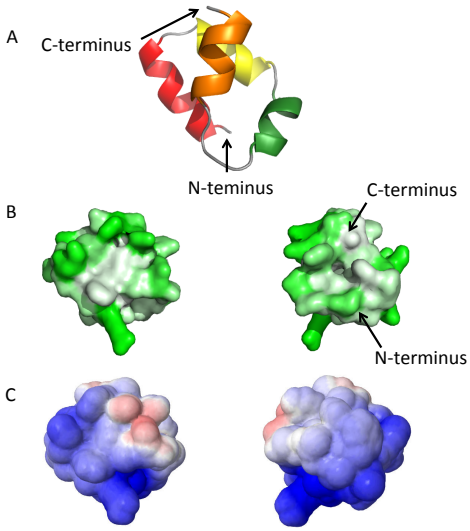

Figure S6- Structural models of mutacin BhtB. A) Ribbon diagram depicting the saposin-like fold. The C- and N- termini are explicitly shown. Hydrophobic surface (B) and electrostatic potential surface (C) maps of mutacin BhtB. Orientation peptide backbone in surface filling diagrams, B and C, correlate to one another.

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